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* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	MAR 15	WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS	3	MAR 16	CASREACT coverage extended
NEWS	4	MAR 20	MARPAT now updated daily
NEWS	5	MAR 22	LWPI reloaded
NEWS	6	MAR 30	RDISCLOSURE reloaded with enhancements
NEWS	7	APR 02	JICST-EPLUS removed from database clusters and STN
NEWS	8	APR 30	GENBANK reloaded and enhanced with Genome Project ID field
NEWS	9	APR 30	CHEMCATS enhanced with 1.2 million new records
NEWS	10	APR 30	CA/CAPplus enhanced with 1870-1889 U.S. patent records
NEWS	11	APR 30	INPADOC replaced by INPADOCDB on STN
NEWS	12	MAY 01	New CAS web site launched
NEWS	13	MAY 08	CA/CAPplus Indian patent publication number format defined
NEWS	14	MAY 14	RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS	15	MAY 21	BIOSIS reloaded and enhanced with archival data
NEWS	16	MAY 21	TOXCENTER enhanced with BIOSIS reload
NEWS	17	MAY 21	CA/CAPplus enhanced with additional kind codes for German patents
NEWS	18	MAY 22	CA/CAPplus enhanced with IPC reclassification in Japanese patents
NEWS	19	JUN 27	CA/CAPplus enhanced with pre-1967 CAS Registry Numbers
NEWS	20	JUN 29	STN Viewer now available
NEWS	21	JUN 29	STN Express, Version 8.2, now available
NEWS	22	JUL 02	LEMBASE coverage updated
NEWS	23	JUL 02	LMEDLINE coverage updated
NEWS	24	JUL 02	SCISEARCH enhanced with complete author names
NEWS	25	JUL 02	CHEMCATS accession numbers revised
NEWS	26	JUL 02	CA/CAPplus enhanced with utility model patents from China
NEWS	27	JUL 16	CAPplus enhanced with French and German abstracts
NEWS	28	JUL 18	CA/CAPplus patent coverage enhanced

NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic:

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 06:26:04 ON 19 JUL 2007

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 06:26:13 ON 19 JUL 2007

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STRUCTURE FILE UPDATES: 18 JUL 2007 HIGHEST RN 942651-59-4

DICTIONARY FILE UPDATES: 18 JUL 2007 HIGHEST RN 942651-59-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

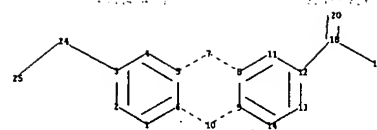
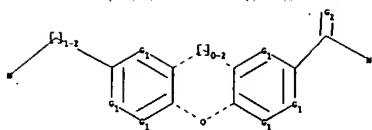
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10598690.str



chain nodes :

18 20 24

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14

ring/chain nodes :

19 25

chain bonds :

3-24 12-18 18-19 18-20 24-25

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-14 11-12 12-13 13-14

exact/norm bonds :

1-2 1-6 2-3 3-4 3-24 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-14 11-12 12-13 12-18 13-14 18-19 18-20 24-25

isolated ring systems :

containing 1 :

G1:C,N

G2:O,N

Match level :

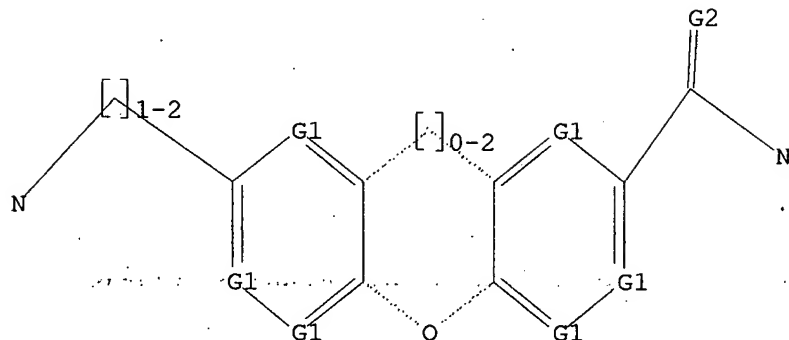
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11:Atom 12:Atom 13:Atom 14:Atom 18:CLASS 19:CLASS 20:CLASS 24:CLASS
25:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 C,N

G2 O,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 06:26:33 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 47839 TO ITERATE

4.2% PROCESSED 2000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 943726 TO 969834

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 06:26:37 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 953477 TO ITERATE

100.0% PROCESSED 953477 ITERATIONS

82 ANSWERS

SEARCH TIME: 00.00.06

L3 82 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

172.10

172.31

FILE 'CAPLUS' ENTERED AT 06:26:51 ON 19 JUL 2007

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FILE COVERS 1907 - 19 Jul 2007 VOL 147 ISS 4
FILE LAST UPDATED: 18 Jul 2007 (20070718/ED)

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=> s l3 full

L4 32 L3

=> d ibib abs hitstr tot

L4 ANSWER 1 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:1042239 CAPLUS

DOCUMENT NUMBER: 143:347068

TITLE: Preparation of dibenzo[b,f]oxepine derivatives as opioid receptor antagonists

INVENTOR(S): Broughton, Howard Barff; Diaz Buezo, Nuria; Mitch, Charles Howard; Pedregal-Tercero, Concepcion

PATENT ASSIGNEE(S): Eli Lilly and Company, USA

SOURCE: PCT Int. Appl., 58 pp.

CODEN: PIXXD2

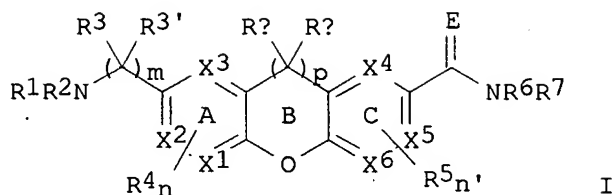
DOCUMENT TYPE: Patent

LANGUAGE: English

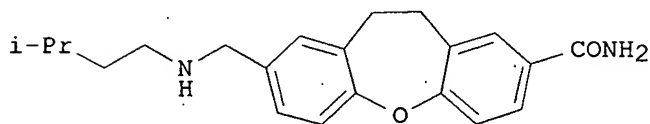
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2558652	A1	20050929	CA 2005-2558652	20050308
EP 1730140	A1	20061213	EP 2005-724568	20050308
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR			
PRIORITY APPLN. INFO.:			EP 2004-380057	A 20040312
			US 2004-553187P	P 20040315
			WO 2005-US7052	W 20050308
OTHER SOURCE(S):	MARPAT 143:347068			
GI				



I



II

AB Title compds. represented by the formula I [wherein X1-X6 = independently C, CH or N; R1, R2 = independently H, alkyl(aryl), alkenyl, etc.; R3, R3' = independently H, alkyl, alkynyl, etc.; Ra, Rb = independently H, alkyl or RaRb = -CH=CH-; R4, R5 = independently H, (halo)alkyl, aryl, etc.; R6, R7 = independently H, alkyl(aryl), alkenyl, etc.; m = 1 or 2; n, n' = independently 0-2; p = 0-2; E = O or NH; and pharmaceutically acceptable salts, solvates, prodrugs, tautomers, enantiomers, racemates, diastereomers and mixture of diastereomers thereof] were prepared as opioid receptor antagonists. For example, II was provided in a multi-step synthesis starting from 10,11-dihydrodibenzo[b,f]oxepine. I were tested for antagonistic activity of μ -, γ - and δ -opioid receptor in SPA-based GTP γ S binding assay, and their pharmaceutical formulations were also presented. Thus, I and their pharmaceutical compns. are useful as opioid receptor antagonists for the treatment of obesity (no data).

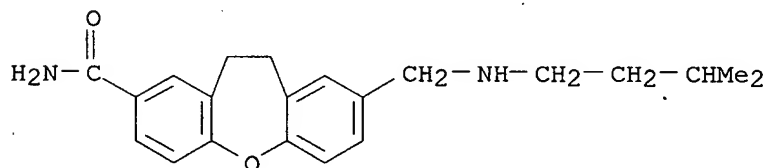
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865539-44-2P 865539-47-5P 865539-55-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of dibenzo[b,f]oxepine derivs. as opioid receptor antagonists)

RN 865538-98-3 CAPLUS

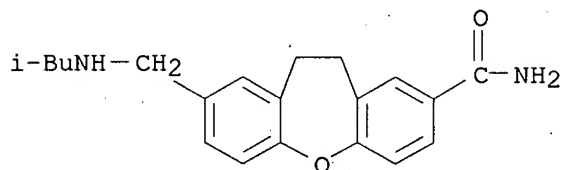
CN Dibenz[b,f]oxepin-2-carboxamide, 10,11-dihydro-8-[[(3-methylbutyl)amino]methyl]- (9CI) (CA INDEX NAME)



RN 865539-01-1 CAPLUS

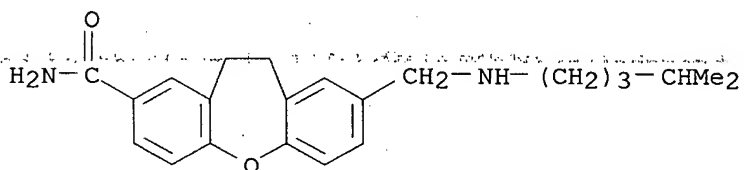
CN Dibenz[b,f]oxepin-2-carboxamide, 10,11-dihydro-8-[[(2-

methylpropyl)amino)methyl]- (9CI) (CA INDEX NAME)



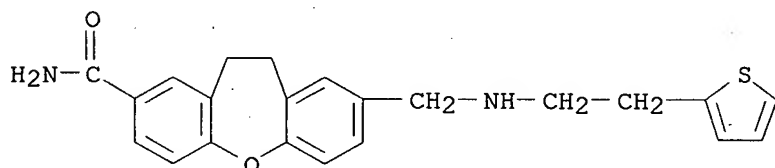
RN 865539-02-2 CAPLUS

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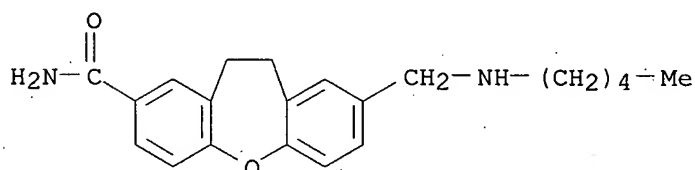
RN 865539-03-3 CAPLUS

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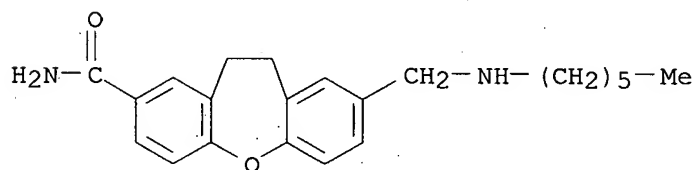
RN 865539-04-4 CAPLUS

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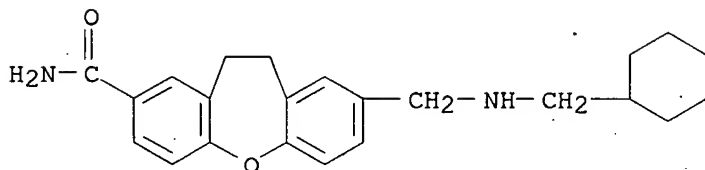
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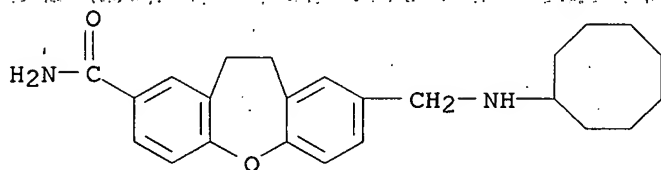
RN 865539-06-6 CAPLUS

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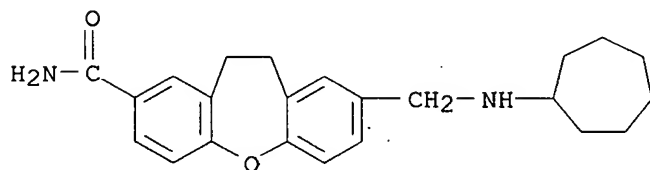
RN 865539-07-7 CAPLUS

CN Dibenz[b,f]oxepin-2-carboxamide, 8-[(cyclooctylamino)methyl]-10,11-dihydro- (9CI) (CA INDEX NAME)



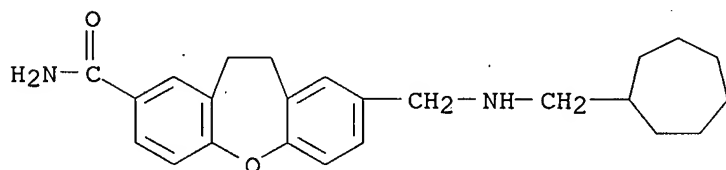
RN 865539-08-8 CAPLUS

CN Dibenz[b,f]oxepin-2-carboxamide, 8-[(cycloheptylamino)methyl]-10,11-dihydro- (9CI) (CA INDEX NAME)



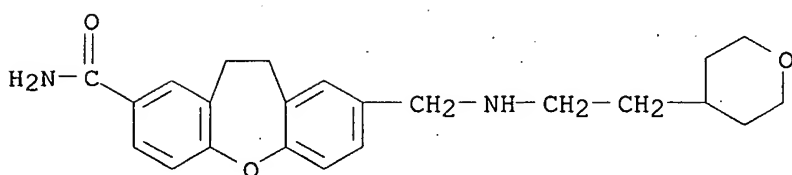
RN 865539-09-9 CAPLUS

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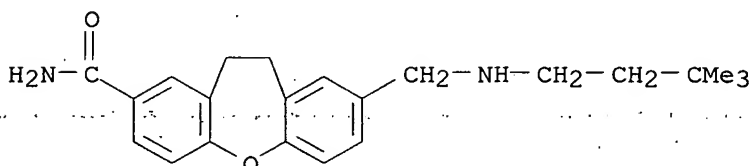


RN 865539-10-2 CAPLUS

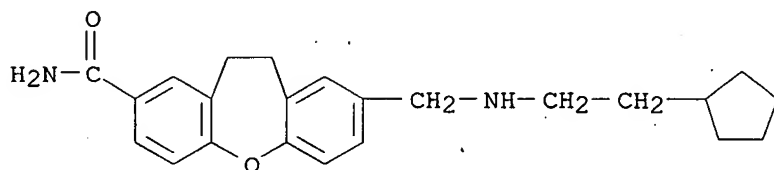
CN Dibenz[b,f]oxepin-2-carboxamide, 10,11-dihydro-8-[[[2-(tetrahydro-2H-pyran-4-yl)ethyl]amino]methyl]- (9CI) (CA INDEX NAME)



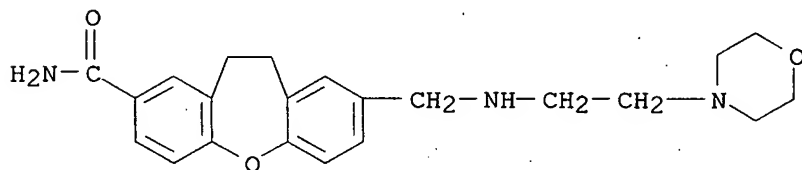
RN 865539-11-3 CAPLUS
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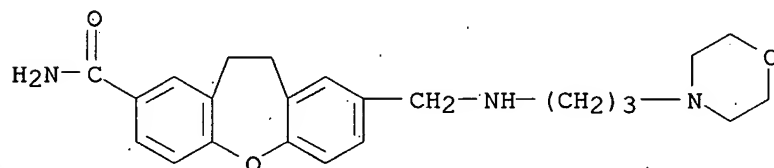
RN 865539-13-5 CAPLUS
 CN Dibenz[b,f]oxepin-2-carboxamide, 8-[[[2-(cyclopentylethyl)amino]methyl]-10,11-dihydro- (9CI) (CA INDEX NAME)



RN 865539-15-7 CAPLUS
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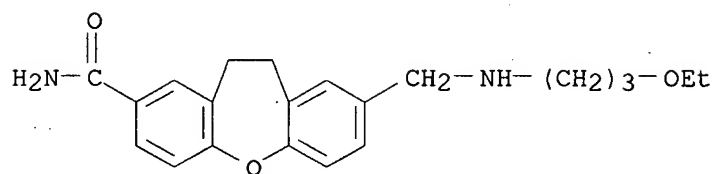


RN 865539-17-9 CAPLUS
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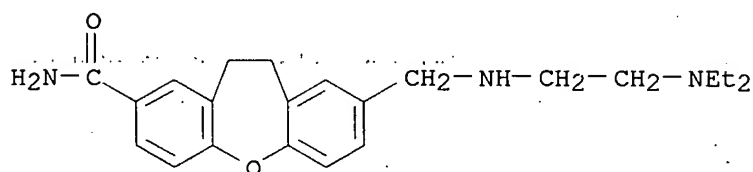
RN 865539-19-1 CAPLUS
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dihydro- (9CI) (CA INDEX NAME)



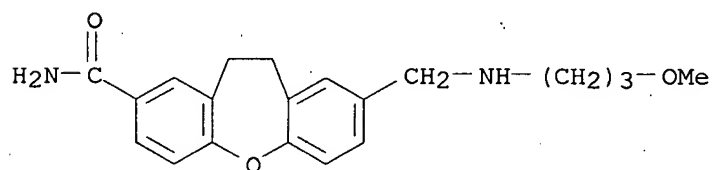
RN 865539-22-6 CAPLUS

CN Dibenz[b,f]oxepin-2-carboxamide, 8-[[[2-(diethylamino)ethyl]amino]methyl]-10,11-dihydro- (9CI) (CA INDEX NAME)



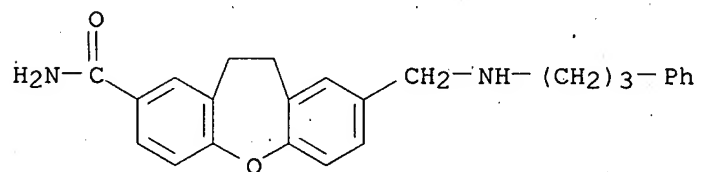
RN 865539-24-8 CAPLUS

CN Dibenz[b,f]oxepin-2-carboxamide, 10,11-dihydro-8-[[[3-methoxypropyl]amino]methyl]- (9CI) (CA INDEX NAME)



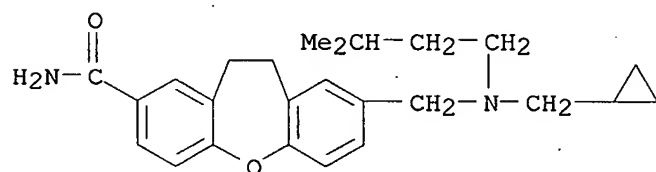
RN 865539-26-0 CAPLUS

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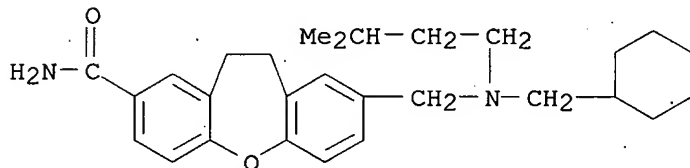


RN 865539-27-1 CAPLUS

CN Dibenz[b,f]oxepin-2-carboxamide, 8-[[[cyclopropylmethyl](3-methylbutyl)amino]methyl]-10,11-dihydro- (9CI) (CA INDEX NAME)



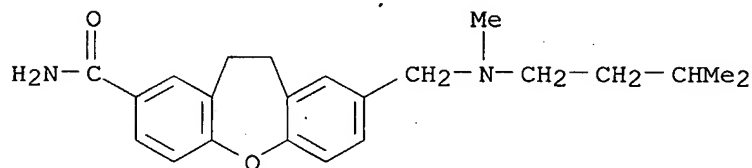
RN 865539-29-3 CAPLUS
 CN Dibenz[b,f]oxepin-2-carboxamide, 8-[[[(cyclohexylmethyl)(3-methylbutyl)amino)methyl]-10,11-dihydro- (9CI) (CA INDEX NAME)



RN 865539-32-8 CAPLUS
 CN Dibenz[b,f]oxepin-2-carboxamide, 10,11-dihydro-8-[[methyl(3-methylbutyl)amino)methyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

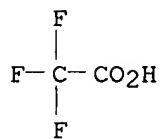
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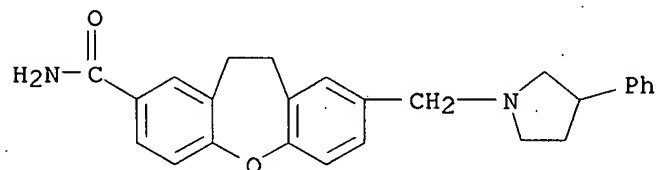


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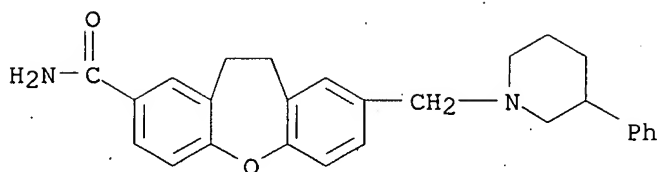
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RN 865539-33-9 CAPLUS
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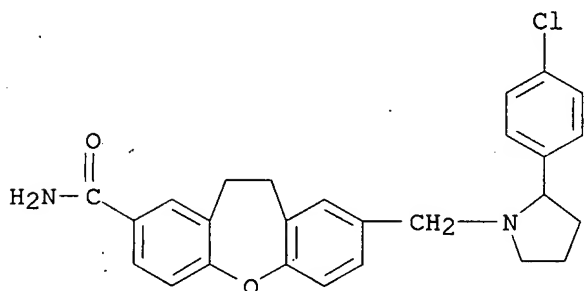


RN 865539-34-0 CAPLUS
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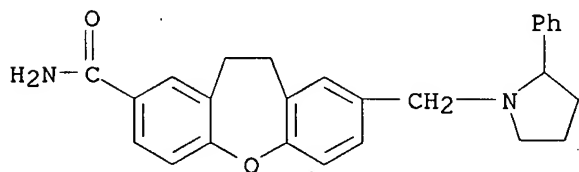
RN 865539-35-1 CAPLUS

CN Dibenzo[b,f]oxepin-2-carboxamide, 8-[[2-(4-chlorophenyl)-1-pyrrolidinyl]methyl]-10,11-dihydro- (9CI) (CA INDEX NAME)



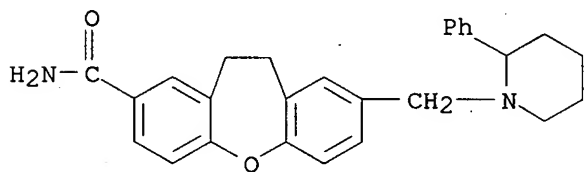
RN 865539-36-2 CAPLUS

CN Dibenzo[b,f]oxepin-2-carboxamide, 10,11-dihydro-8-[(2-phenyl-1-pyrrolidinyl)methyl]- (9CI) (CA INDEX NAME)



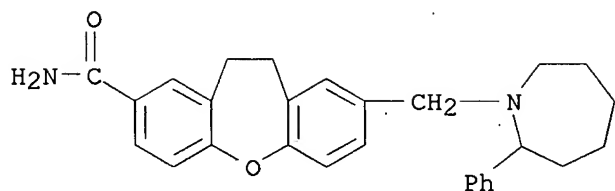
RN 865539-37-3 CAPLUS

CN Dibenzo[b,f]oxepin-2-carboxamide, 10,11-dihydro-8-[(2-phenyl-1-piperidiny]methyl]- (9CI) (CA INDEX NAME)



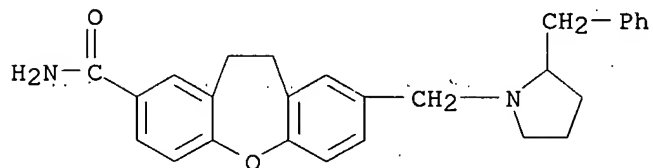
RN 865539-38-4 CAPLUS

CN Dibenzo[b,f]oxepin-2-carboxamide, 8-[(hexahydro-2-phenyl-1H-azepin-1-yl)methyl]-10,11-dihydro- (9CI) (CA INDEX NAME)



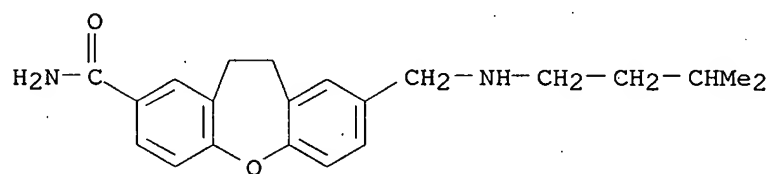
RN 865539-39-5 CAPLUS

CN Dibenzo[b,f]oxepin-2-carboxamide, 10,11-dihydro-8-[[2-(phenylmethyl)-1-pyrrolidinyl]methyl]- (9CI) (CA INDEX NAME)



RN 865539-40-8 CAPLUS

CN Dibenzo[b,f]oxepin-2-carboxamide, 10,11-dihydro-8-[[3-methylbutyl]amino]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

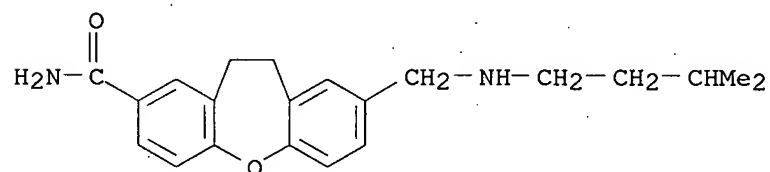
RN 865539-41-9 CAPLUS

CN Dibenzo[b,f]oxepin-2-carboxamide, 10,11-dihydro-8-[[3-methylbutyl]amino]methyl]-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 865538-98-3

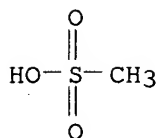
CMF C21 H26 N2 O2



CM 2

CRN 75-75-2

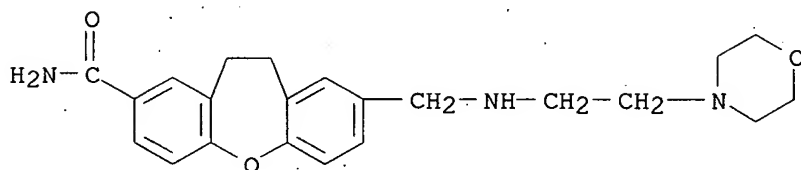
CMF C H4 O3 S



RN 865539-42-0 CAPLUS
 CN Dibenz[b,f]oxepin-2-carboxamide, 10,11-dihydro-8-[[[2-(4-morpholinyl)ethyl]amino]methyl]-, dimethanesulfonate (9CI) (CA INDEX NAME)

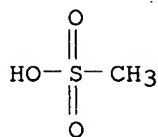
CM 1

CRN 865539-15-7
 CMF C22 H27 N3 O3



CM 2

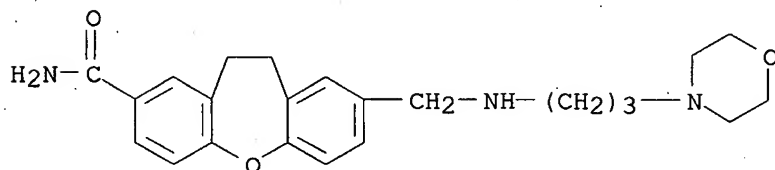
CRN 75-75-2
 CMF C H4 O3 S



RN 865539-43-1 CAPLUS
 CN Dibenz[b,f]oxepin-2-carboxamide, 10,11-dihydro-8-[[[3-(4-morpholinyl)propyl]amino]methyl]-, dimethanesulfonate (9CI) (CA INDEX NAME)

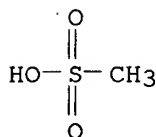
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CRN 865539-17-9
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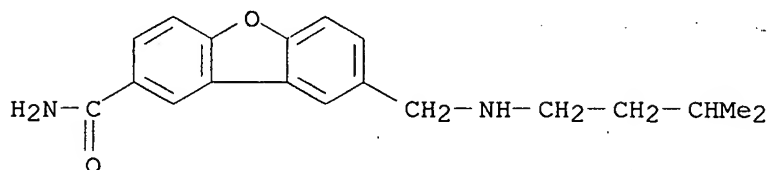


CM 2

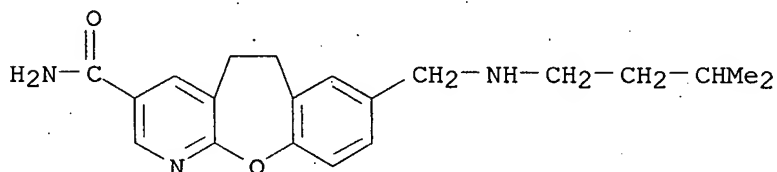
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CMF C H4 O3 S



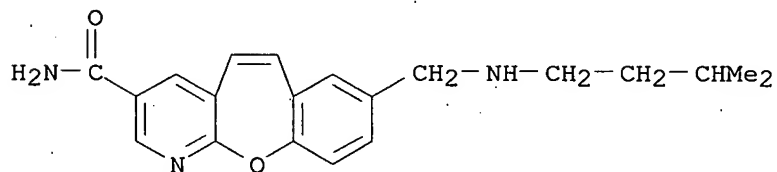
RN 865539-44-2 CAPLUS
CN 2-Dibenzofurancarboxamide, 8-[[(3-methylbutyl) amino]methyl]- (9CI) (CA INDEX NAME)



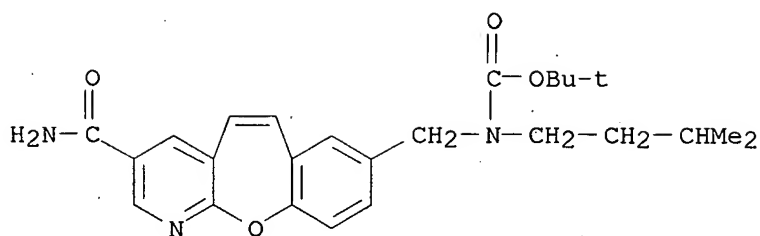
RN 865539-47-5 CAPLUS
CN [1]Benzoxepino[2,3-b]pyridine-3-carboxamide, 5,6-dihydro-8-[[(3-methylbutyl) amino]methyl]- (9CI) (CA INDEX NAME)



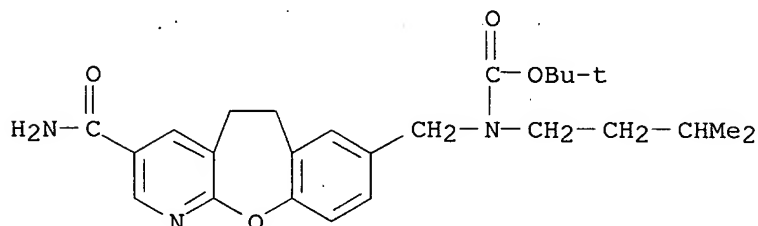
RN 865539-55-5 CAPLUS
CN [1]Benzoxepino[2,3-b]pyridine-3-carboxamide, 8-[[(3-methylbutyl) amino]methyl]- (9CI) (CA INDEX NAME)



IT 865539-53-3P 865539-54-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of dibenzo[b,f]oxepine derivs. as opioid receptor antagonists)
RN 865539-53-3 CAPLUS
CN Carbamic acid, [[3-(aminocarbonyl)[1]benzoxepino[2,3-b]pyridin-8-yl]methyl](3-methylbutyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 865539-54-4 CAPLUS
 CN Carbamic acid, [[3-(aminocarbonyl)-5,6-dihydro[1]benzoxepino[2,3-b]pyridin-8-yl]methyl](3-methylbutyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:216611 CAPLUS
 DOCUMENT NUMBER: 142:291340
 TITLE: Formulations, conjugates, and combinations of drugs for the treatment of neoplasms
 INVENTOR(S): Nichols, James M.; Foley, Michael A.; Keith, Curtis; Padval, Mahesh; Elliott, Peter
 PATENT ASSIGNEE(S): Combinatorx, Incorporated, USA
 SOURCE: PCT Int. Appl., 92 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005020913	A2	20050310	WO 2004-US27695	20040825
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005080075	A1	20050414	US 2004-925835	20040825
PRIORITY APPLN. INFO.:			US 2003-497617P	P 20030825
OTHER SOURCE(S): MARPAT 142:291340				
AB The invention provides formulations and structural modifications for				

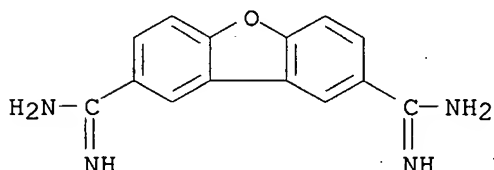
phenothiazine compds. which result in altered biodistribution, thereby reducing the occurrence of adverse reactions associated with this class of drug.

IT 338945-24-7, 2,8-Dibenzofurandicarboximidamide 415718-17-1
415718-20-6

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
(formulations and conjugates and combinations of drugs such as
phenothiazines for treatment of neoplasms)

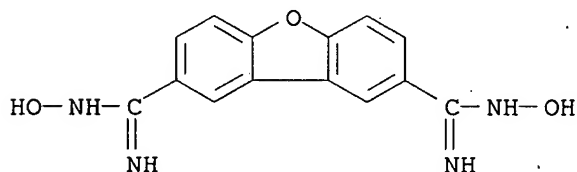
RN 338945-24-7 CAPLUS

CN 2,8-Dibenzofurandicarboximidamide (9CI) (CA INDEX NAME)



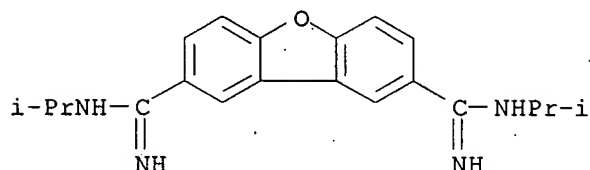
RN 415718-17-1 CAPLUS

CN 2,8-Dibenzofurandicarboximidamide, N,N''-dihydroxy- (9CI) (CA INDEX NAME)



RN 415718-20-6 CAPLUS

CN 2,8-Dibenzofurandicarboximidamide, N,N''-bis(1-methylethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:120654 CAPLUS

DOCUMENT NUMBER: 142:191226

TITLE: Combination of pentamidine or analog and
antiproliferative agent drugs for the treatment of
neoplasms

INVENTOR(S): Nichols, James M.; Lee, Margaret S.; Keith, Curtis T.;
Zhang, Yanzhen; Gaw, Debra A.

PATENT ASSIGNEE(S): Combinatorx, Incorporated, USA

SOURCE: PCT Int. Appl., 71 pp.

CODEN: PIXXD2

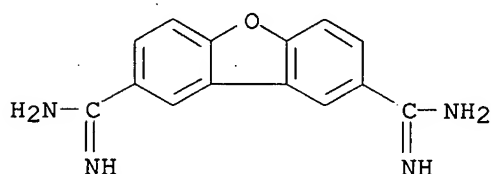
DOCUMENT TYPE: Patent

LANGUAGE: English

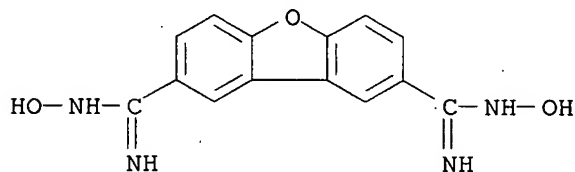
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

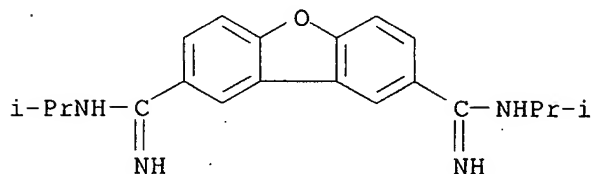
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005011572	A2	20050210	WO 2004-US23524	20040722
WO 2005011572	A3	20050310		
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US 2005054708	A1	20050310	US 2004-895561	20040721
AU 2004261148	A1	20050210	AU 2004-261148	20040722
CA 2529521	A1	20050210	CA 2004-2529521	20040722
EP 1651211	A2	20060503	EP 2004-778848	20040722
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK CN 1829509 A 20060906 CN 2004-80022015 20040722 JP 2007500698 T 20070118 JP 2006-521916 20040722 PRIORITY APPLN. INFO.: US 2003-490759P P 20030728 WO 2004-US23524 W 20040722				
OTHER SOURCE(S): MARPAT 142:191226				
AB The invention features a method for treating a patient having a cancer or other neoplasm by administering to the patient pentamidine or a pentamidine analog and an antiproliferative agent simultaneously or within 14 days of each other in amts. sufficient to treat the patient. The combination of pentamidine and vinblastine provided improved antiproliferative activity against human non-small cell lung carcinoma A549 cells.				
IT 338945-24-7, 2,8-Dibenzofurandicarboximidamide 415718-17-1 415718-20-6 RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (combination of pentamidine or analog and antiproliferative agent drugs for treatment of neoplasms)				
RN 338945-24-7 CAPLUS CN 2,8-Dibenzofurandicarboximidamide (9CI) (CA INDEX NAME)				



RN 415718-17-1 CAPLUS
 CN 2,8-Dibenzofurandicarboximidamide, N,N''-dihydroxy- (9CI) (CA INDEX NAME)



RN 415718-20-6 CAPLUS
CN 2,8-Dibenzofurandicarboximidamide, N,N''-bis(1-methylethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 4 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:60255 CAPLUS

DOCUMENT NUMBER: 140:105258

TITLE: Benzimidazole compound-pentamidine compound

combinations for the treatment of neoplasms

INVENTOR(S): Borisy, Alexis; Keith, Curtis; Foley, Michael A.;
Stockwell, Brent R.; Gaw, Debra A.

PATENT ASSIGNEE(S): Combinatorx, Incorporated, USA

SOURCE: PCT Int. Appl., 79 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004006849	A2	20040122	WO 2003-US21984	20030715
WO 2004006849	A3	20040603		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2003251904	A1	20040202	AU 2003-251904	20030715
PRIORITY APPLN. INFO.:			US 2002-396151P	P 20020715
			WO 2003-US21984	W 20030715

OTHER SOURCE(S): MARPAT 140:105258

AB The invention features a method for treating a patient having a cancer or other neoplasm, by administering to the patient (i) a benzimidazole or a metabolite or analog thereof; and (ii) pentamidine or a metabolite or analog thereof simultaneously or within 14 days of each other in amts. sufficient to inhibit the growth of the neoplasm.

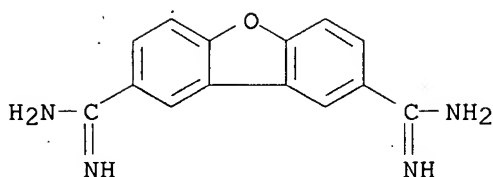
IT 338945-24-7, 2,8-Dibenzofurandicarboximidamide 415718-17-1
415718-20-6

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(benzimidazole compound-pentamidine compound combinations for the treatment of neoplasms)

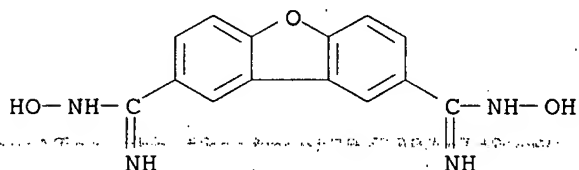
RN 338945-24-7 CAPLUS

CN 2,8-Dibenzofurandicarboximidamide (9CI) (CA INDEX NAME)



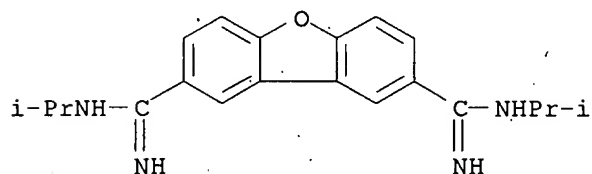
RN 415718-17-1 CAPLUS

CN 2,8-Dibenzofurandicarboximidamide, N,N''-dihydroxy- (9CI) (CA INDEX NAME)



RN 415718-20-6 CAPLUS

CN 2,8-Dibenzofurandicarboximidamide, N,N''-bis(1-methylethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 5 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:60249 CAPLUS

DOCUMENT NUMBER: 140:122767

TITLE: Pentamidine compound-chlorpromazine compound combinations for the treatment of neoplasms

INVENTOR(S): Borisy, Alexis; Keith, Curtis; Foley, Michael A.; Stockwell, Brent R.; Gaw, Debra A.; Nichols, M. James; Lee, Margaret S.

PATENT ASSIGNEE(S): Combinatorx, Incorporated, USA

SOURCE: PCT Int. Appl., 76 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004006842	A2	20040122	WO 2003-US21803	20030711
WO 2004006842	A3	20040527		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,

FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2492059	A1	20040122	CA 2003-2492059	20030711
AU 2003256511	A1	20040202	AU 2003-256511	20030711
US 2004116407	A1	20040617	US 2003-617424	20030711
BR 2003012597	A	20050510	BR 2003-12597	20030711
EP 1545544	A2	20050629	EP 2003-764557	20030711
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1681511	A	20051012	CN 2003-821151	20030711
JP 2005536509	T	20051202	JP 2004-521730	20030711
MX 2005PA00485	A	20050419	MX 2005-PA485	20050111
NO 2005000204	A	20050408	NO 2005-204	20050113
IN 2005CN00160	A	20070330	IN 2005-CN160	20050210
US 2007099905	A1	20070503	US 2006-585486	20061024
PRIORITY APPLN. INFO.:			US 2002-395233P	P 20020711
			US 2003-617424	A1 20030711
			WO 2003-US21803	W 20030711

OTHER SOURCE(S): MARPAT-140:122767

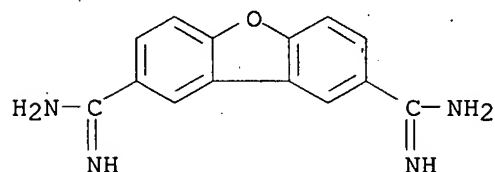
AB The invention features a method for treating a patient having a cancer or other neoplasm by administering to the patient pentamidine (or an analog thereof) and chlorpromazine (or an analog thereof) simultaneously or within 14 days of each other in amts. sufficient to treat the patient.

IT 338945-24-7, 2,8-Dibenzofurandicarboximidamide 415718-17-1
 415718-20-6

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
 (Biological study); USES (Uses)
 (pentamidine compound-chlorpromazine compound combinations for the
 treatment of neoplasms)

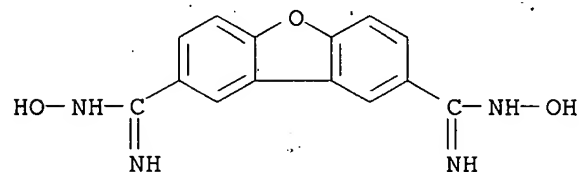
RN 338945-24-7 CAPLUS

CN 2,8-Dibenzofurandicarboximidamide (9CI) (CA INDEX NAME)



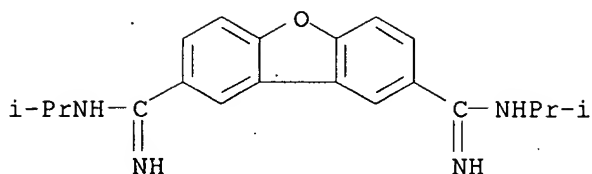
RN 415718-17-1 CAPLUS

CN 2,8-Dibenzofurandicarboximidamide, N,N''-dihydroxy- (9CI) (CA INDEX NAME)



RN 415718-20-6 CAPLUS

CN 2,8-Dibenzofurandicarboximidamide, N,N''-bis(1-methylethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 6 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:146280 CAPLUS

DOCUMENT NUMBER: 136:321920

TITLE: Antileishmanial activities of several classes of aromatic dications

AUTHOR(S): Brendle, James J.; Outlaw, Abram; Kumar, Arvind; Boykin, David W.; Patrick, Donald A.; Tidwell, Richard R.; Werbovetz, Karl A.

CORPORATE SOURCE: Division of Experimental Therapeutics, Walter Reed Army Institute of Research, Silver Spring, MD, 20910, USA

SOURCE: Antimicrobial Agents and Chemotherapy (2002), 46(3), 797-807

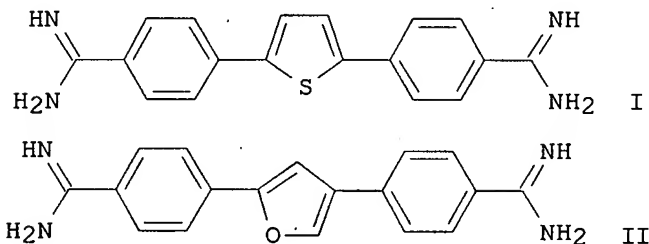
CODEN: AMACCO; ISSN: 0066-4804

PUBLISHER: American Society for Microbiology

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Aromatic dicationic mols. possess impressive activity against a broad spectrum of microbial pathogens, including *Pneumocystis carinii*, *Cryptosporidium parvum*, and *Candida albicans*. In this work, 58 aromatic cations were examined for inhibitory activity against axenic amastigote-like *Leishmania donovani* parasites. In general, the most potent of the compds. were substituted di-Ph furan and thiophene dications. 2,5-Bis-(4-amidinophenyl)thiophene (I) was the most active compound. This agent displayed a 50% inhibitory concentration (IC₅₀) of $0.42 \pm 0.08 \mu\text{M}$ against *L. donovani* and an in vitro antileishmanial potency 6.2-fold greater than that of the clin. antileishmanial dication pentamidine and was 155-fold more toxic to the parasites than to a mouse macrophage cell line. 2,4-Bis-(4-amidinophenyl)furan (II) was twice as active as pentamidine (IC₅₀, $1.30 \pm 0.21 \mu\text{M}$), while 2,5-bis-(4-amidinophenyl)furan and pentamidine were essentially equipotent in our in vitro antileishmanial assay. Carbazoles, dibenzofurans, dibenzothiophenes, and benzimidazoles containing amidine or substituted amidine groups were generally less active than the di-Ph furans and thiophenes. In all cases, aromatic dications possessing strong antileishmanial activity were several-fold more toxic to the parasites than to a cultured mouse macrophage cell line. These structure-activity relationships demonstrate the potent antileishmanial activity of several

aromatic dications and provide valuable information for the future design and synthesis of more potent antiparasitic agents.

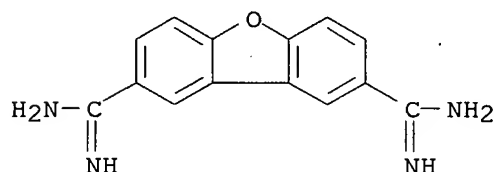
IT 338945-24-7, 2,8-Dibenzofurandicarboximidamide 415718-17-1
415718-20-6

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(antileishmanial activities of several classes of aromatic dications)

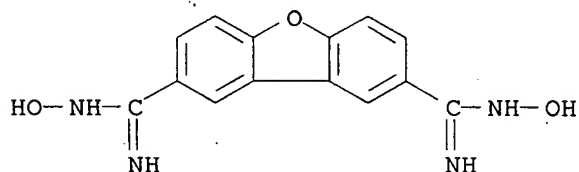
RN 338945-24-7 CAPLUS

CN 2,8-Dibenzofurandicarboximidamide (9CI) (CA INDEX NAME)



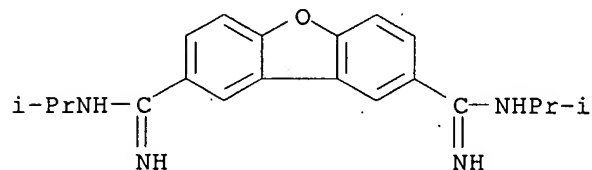
RN 415718-17-1 CAPLUS

CN 2,8-Dibenzofurandicarboximidamide, N,N''-dihydroxy- (9CI) (CA INDEX NAME)



RN 415718-20-6 CAPLUS

CN 2,8-Dibenzofurandicarboximidamide, N,N''-bis(1-methylethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:850947 CAPLUS

DOCUMENT NUMBER: 136:689

TITLE: Coumermycin analogs, their preparation, and their use as chemical dimerizers of chimeric proteins

INVENTOR(S): Farrar, Michael A.; Olson, Steven H.; Perlmutter, Roger M.; Slossberg, Llnon H.

PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: PCT Int. Appl., 54 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.

KIND DATE

APPLICATION NO.

DATE

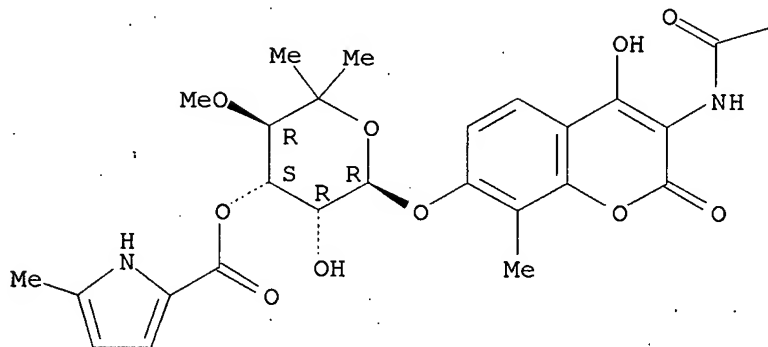
WO 2001087309	A1	20011122	WO 2001-US14870	20010508
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002095026	A1	20020718	US 2001-840260	20010423
US 6916846	B2	20050712		
PRIORITY APPLN. INFO.:			US 2000-203656P	P. 20000512
OTHER SOURCE(S):			MARPAT 136:689	
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

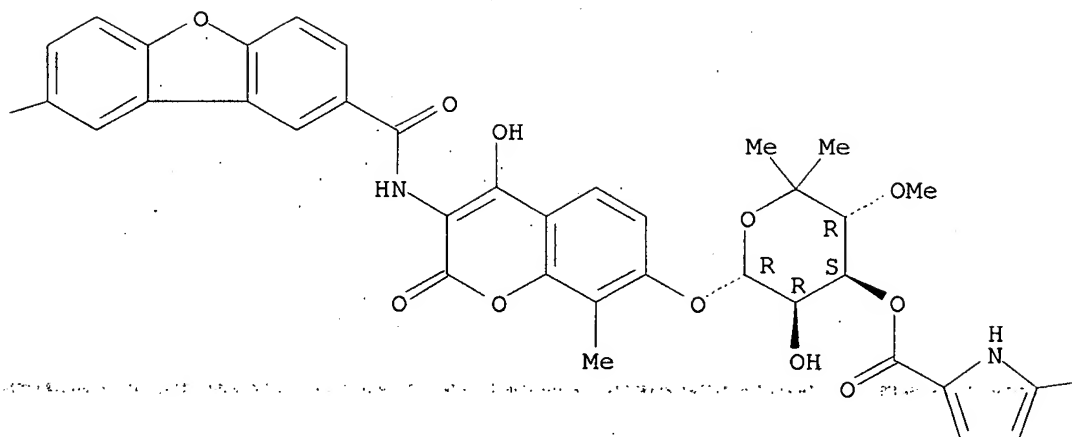
- AB Coumermycin analogs I (X = alkyl, aryl, diaryl, substituted alkyl, substituted aryl, alkyl with heteroatoms in chain, heteroaryl, cyclic and bicyclic alkyl, combination of alkyl, aryl and heteroaryl substituents). The compds. are suitable for use as chemical dimerizers of chimeric proteins. The coumermycin analogs of the invention are useful as chemical dimerizers of chimeric protein kinases or transcription factors. The analogs are capable of covalently attaching the carboxyl terminus of Raf-1 serine/threonine kinase to the amino terminus of the B subunit of bacterial DNA gyrase.
- IT 374749-33-4 374749-33-4D, esters
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (coumermycin analog preparation and use as chemical dimerizers of chimeric proteins)
- RN 374749-33-4 CAPLUS
- CN 2,8-Dibenzofurandicarboxamide, N,N'-bis[7-[[6-deoxy-5-C-methyl-4-O-methyl-3-O-[(5-methyl-1H-pyrrol-2-yl)carbonyl]- α -L-lyxo-hexopyranosyl]oxy]-4-hydroxy-8-methyl-2-oxo-2H-1-benzopyran-3-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



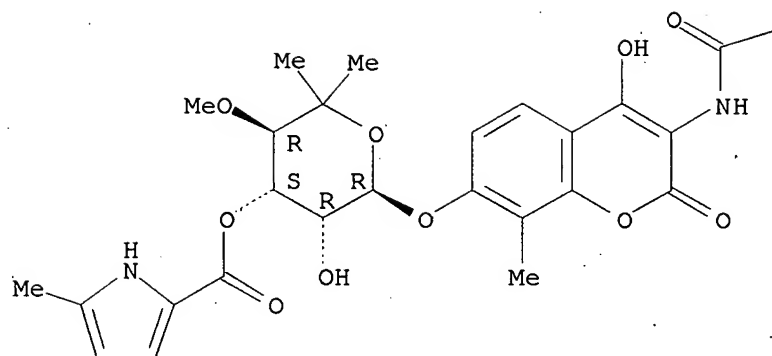
PAGE 1-C

—Me

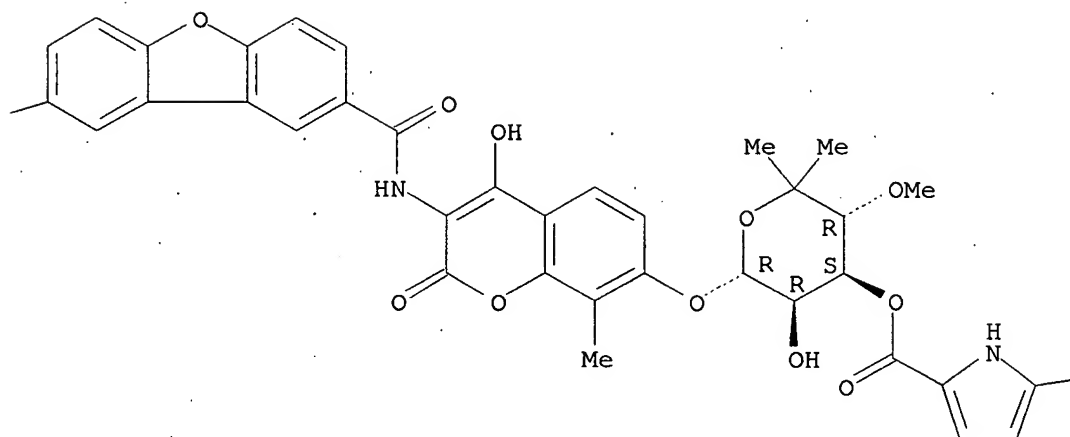
RN 374749-33-4 CAPLUS
CN 2,8-Dibenzofurandicarboxamide, N,N'-bis[7-[[6-deoxy-5-C-methyl-4-O-methyl-3-O-[(5-methyl-1H-pyrrol-2-yl)carbonyl]-α-L-lyxo-hexopyranosyl]oxy]-4-hydroxy-8-methyl-2-oxo-2H-1-benzopyran-3-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



PAGE 1-C

— Me

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS

L4 ANSWER 8 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:338336 CAPLUS

DOCUMENT NUMBER: 134:348244

TITLE: Methods and formulations using heterocyclic compounds for the treatment of infectious bursal disease in avian subjects

INVENTOR(S): Dykstra, Christine C.; Hudson, James C.; Tidwell, Richard R.; Boykin, David; Ewald, Sandra

PATENT ASSIGNEE(S): The University of North Carolina at Chapel Hill, USA; Auburn University; Georgia State University Research Foundation, Inc.

SOURCE: PCT Int. Appl., 58 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001032159	A2	20010510	WO 2000-US30066	20001101
WO 2001032159	A3	20020711		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6774144	B1	20040810	US 2000-703804	20001101
PRIORITY APPLN. INFO.:			US 1999-162877P	P 19991101
OTHER SOURCE(S):			MARPAT 134:348244	

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A method is provided for treating infectious bursal disease (IBD) in an avian subject in need of such treatment. The method comprises administering to the subject a compound of formulas I-IV [p = 1-8; A = O, S, NR (R = H, lower alkyl); X1, X2 = H, lower alkyl, lower alkoxy; R1, R2, X', X'', X3-X6 = lower alkyl, lower alkoxy, aryl, halo, etc.], or a pharmaceutically acceptable salt thereof, in an amount sufficient to treat IBD. In another aspect, the invention provides a method of producing active immunity against infectious bursal virus disease (IBD) in an avian subject. The method comprises administering to a subject an immunogenic-amount of an IBDV vaccine and a compound selected from compds. I-IV. A compound represented by I-IV is administered in an amount sufficient to induce an immune response in the avian subject.

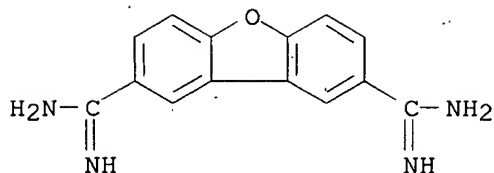
IT 338945-24-7, SW 066

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(heterocyclic compds. for treatment of infectious bursal disease in avians)

RN 338945-24-7 CAPLUS

CN 2,8-Dibenzofurandicarboximidamide (9CI) (CA INDEX NAME)



L4 ANSWER 9 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:144873 CAPLUS

DOCUMENT NUMBER: 132:180475

TITLE: Preparation of bis(amidino)dibenzofurans and
-thiophenes for treating Pneumocystis carinii
pneumonia

INVENTOR(S): Tidwell, Richard R.; Hall, James Edwin

PATENT ASSIGNEE(S): University of North Carolina at Chapel Hill, USA

SOURCE: PCT Int. Appl., 58 pp.

CODEN: PIXXD2

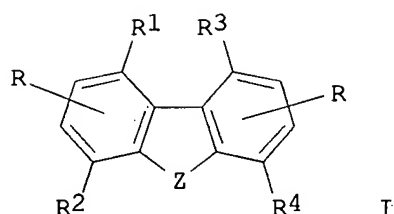
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000010990	A2	20000302	WO 1999-US14313	19990624
WO 2000010990	A3	20030417		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2340912	A1	20000302	CA 1999-2340912	19990624
AU 9947152	A1	20000314	AU 1999-47152	19990624
AU 758563	B2	20030327		
US 6172104	B1	20010109	US 1999-344143	19990624
EP 1105381	A1	20010613	EP 1999-930662	19990624
EP 1105381	B1	20030502		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
AT 239003	T	20030515	AT 1999-930662	19990624
JP 2003523927	T	20030812	JP 2000-566263	19990624
ES 2198139	T3	20040116	ES 1999-930662	19990624
PRIORITY APPLN. INFO.:				
			US 1998-97273P	P 19980820
			WO 1999-US14313	W 19990624
OTHER SOURCE(S): MARPAT 132:180475				
GI				



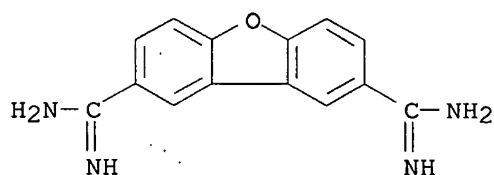
AB Title compds. [I; R independently = H, alkyl, alkoxy, C(:NR5)NR5R6; R1-R4 = H, halo, alkyl, alkoxy, etc.; R5 = H, alkyl, alkoxy, aryl, etc.; R5R5 = alkylene, etc.; R6 = H, OH, alkyl, alkoxy, etc.; Z = O or S] were prepared. Thus, 2,8-dicyanodibenzothiophene was treated with HCl/EtOH and the diimide product treated with NH3EtOH to give 2,8-bis(amidino)dibenzothiophene dihydrochloride. Data for biol. activity of I were given.

IT 232940-74-8P 232940-76-0P 232940-77-1P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of bis(amidino)dibenzofurans and -thiophenes for treating *Pneumocystis carinii* pneumonia)

RN 232940-74-8 CAPLUS

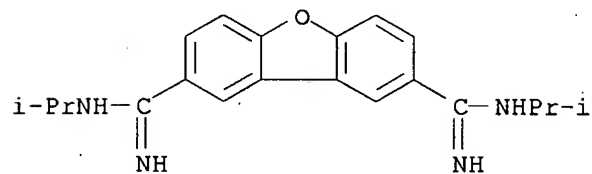
CN 2,8-Dibenzofurandicarboximidamide, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

RN 232940-76-0 CAPLUS

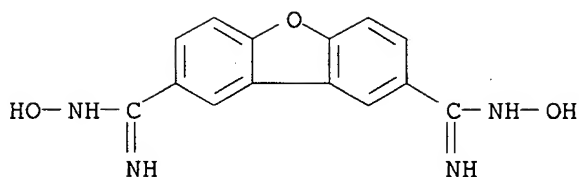
CN 2,8-Dibenzofurandicarboximidamide, N,N''-bis(1-methylethyl)-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

RN 232940-77-1 CAPLUS

CN 2,8-Dibenzofurandicarboximidamide, N,N''-dihydroxy-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

L4 ANSWER 10 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:314005 CAPLUS

DOCUMENT NUMBER: 131:110896

TITLE: Dicationic dibenzofuran derivatives as

anti-Pneumocystis carinii pneumonia agents: synthesis, DNA binding affinity, and anti-P. carinii activity in an immunosuppressed rat model

AUTHOR(S): Wang, Sihe; Hall, James Edwin; Tanious, Farial A.; Wilson, W. David; Patrick, Donald A.; McCurdy, Donald R.; Bender, Brenden C.; Tidwell, Richard R.

CORPORATE SOURCE: Division of Medicinal Chemistry and Natural Products, The University of North Carolina at Chapel Hill, Chapel Hill, NC, 27599, USA

SOURCE: European Journal of Medicinal Chemistry (1999), 34(3), 215-224

CODEN: EJMCA5; ISSN: 0223-5234

PUBLISHER: Editions Scientifiques et Medicales Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Previous work from the authors' laboratory shows that compds. with two cations linked by a carbazole spacer were highly potent anti-P. carinii agents. A prodrug approach designed to increase oral activity of the dicationic carbazoles by converting amidine groups to amidoxime groups was unsuccessful. The ring nitrogen was implicated as playing a role in the lack of activity of carbazole amidoximes. The current study was designed to determine if replacement of the carbazole ring nitrogen by isosteric oxygen to form dibenzofurans would improve effectiveness of amidoxime prodrugs. Eight dibenzofuran dicationic derivs. were synthesized and evaluated for anti-P. carinii activity in an immunosuppressed rat model. Since DNA binding has been hypothesized to play a key role in antimicrobial activity of dicationic compds., the compds. were examined for their binding affinity to calf thymus DNA and a poly-dA-poly-dT oligomer. While several of the compds. were more potent anti-P. carinii agents than pentamidine, the corresponding amidoximes were significantly less effective than the amidoxime of pentamidine. No direct quant. correlation was determined between DNA binding affinity and anti-P. carinii activity, but all active compds. were strong DNA binding agents.

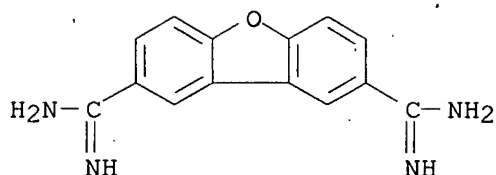
IT 232940-74-8P 232940-76-0P 232940-77-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation, structure and DNA binding of dicationic dibenzofuran derivs. as anti-Pneumocystis carinii pneumonia agents)

RN 232940-74-8 CAPLUS

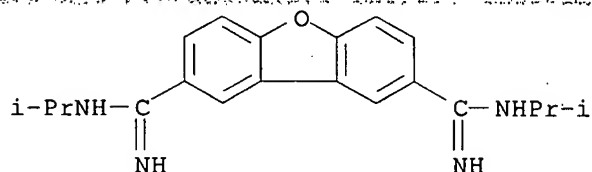
CN 2,8-Dibenzofurandicarboximidamide, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 232940-76-0 CAPLUS

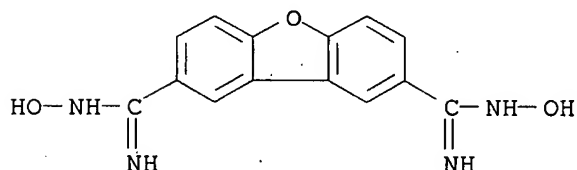
CN 2,8-Dibenzofurandicarboximidamide, N,N''-bis(1-methylethyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 232940-77-1 CAPLUS

CN 2,8-Dibenzofurandicarboximidamide, N,N''-dihydroxy-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:599851 CAPLUS

DOCUMENT NUMBER: 123:102049

TITLE: New promise in combinatorial chemistry: Synthesis, characterization, and screening of small-molecule libraries in solution

AUTHOR(S): Carell, Thomas; Wintner, Edward A.; Sutherland, Andrew J.; Rebek, Julius, Jr.; Dunayevskiy, Yuriy M.; Vouros, Paul

CORPORATE SOURCE: Department Chemistry, Massachusetts Institute Technology, Cambridge, MA, 02139, USA

SOURCE: Chemistry & Biology (1995), 2(3), 171-83
CODEN: CBOLE2; ISSN: 1074-5521

DOCUMENT TYPE: Journal
LANGUAGE: English

AB The increasing interest in combinatorial chemical as a tool for the development of therapeutics has led to many new methods of creating mol. libraries of potential lead compds. Current methods have made it possible to develop libraries of several million compds. As a result, the limiting factor in the screening of libraries has become the identification and characterization of active species. The authors have recently described a method for generating libraries of water-soluble compds. containing mixts. of

104

to 105 different small organic mols. by using generally applicable solution phase chemical. The authors set out to develop new methods to characterize and decode these libraries. Libraries were generated by condensing a multi-acid-chloride core mol. with various amines, producing mols. with functional groups about a rigid backbone. Composition and complexity of the libraries was evaluated using electrospray mass spectrometry to analyze model libraries containing ≤ 55 different mols. The number of peaks obtained in mass spectrometry is directly correlated with the complexity of the library, and the authors were therefore able to deduce which of the expected compds. had in fact been formed in the library, and which of the building blocks in the library were not efficiently used. An iterative selection procedure was developed using this information, which allowed the screening of libraries of $\leq 50,000$ chemical species to produce a competitive inhibitor of the enzyme trypsin. The authors' strategy for the identification of active species should be broadly applicable to other methods of generating complex libraries of small mols. The selection from the library of a compound with desired biol. properties augurs well for the potential value of generating and screening complex mixts. of small mols. in solution

IT 166034-37-3P 166034-38-4P

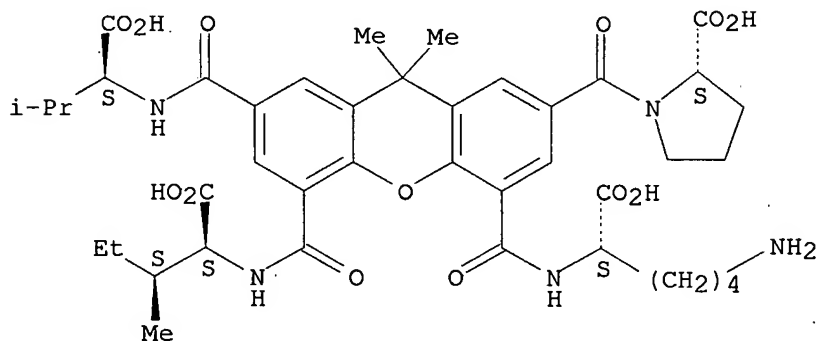
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(new promise in combinatorial chemical in relation to synthesis and characterization and pharmacol. screening of small-mol. libraries in solution as trypsin inhibitors)

RN 166034-37-3 CAPLUS

CN L-Proline, 1-[[4-[[[(5-amino-1-carboxypentyl)amino]carbonyl]-5-[[[(1-carboxy-2-methylbutyl)amino]carbonyl]-7-[[[(1-carboxy-2-methylpropyl)amino]carbonyl]-9,9-dimethyl-9H-xanthen-2-yl]carbonyl]-, stereoisomer (9CI) (CA INDEX NAME)

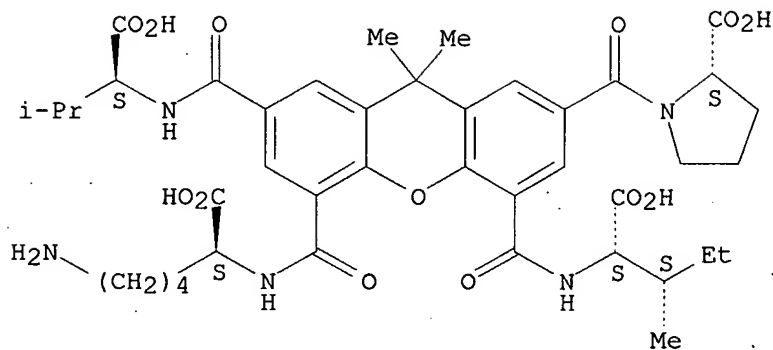
Absolute stereochemistry.



RN 166034-38-4 CAPLUS

CN L-Proline, 1-[[5-[[[(5-amino-1-carboxypentyl)amino]carbonyl]-4-[[[(1-carboxy-2-methylbutyl)amino]carbonyl]-7-[[[(1-carboxy-2-methylpropyl)amino]carbonyl]-9,9-dimethyl-9H-xanthen-2-yl]carbonyl]-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 166034-35-1P 166034-36-2P

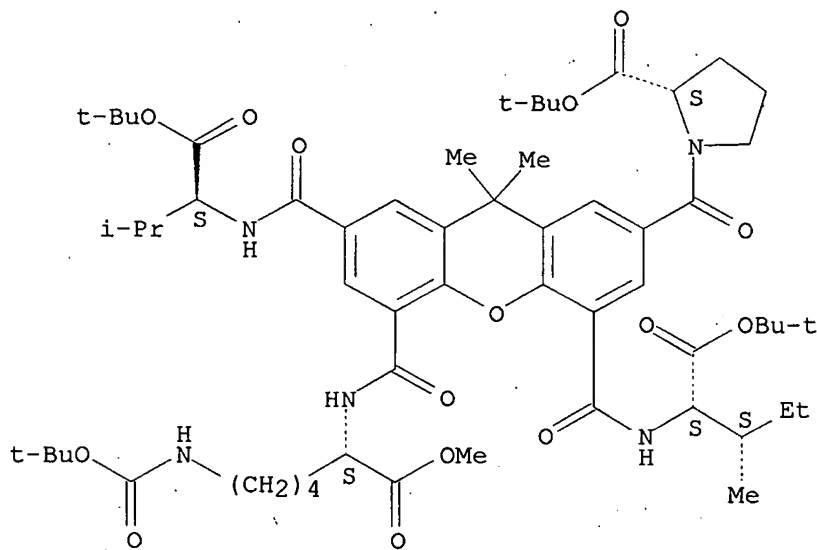
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(new promise in combinatorial chemical in relation to synthesis and characterization and pharmacol. screening of small-mol. libraries in solution as trypsin inhibitors)

RN 166034-35-1 CAPLUS

CN L-Proline, 1-[[[5-[[[5-[[[1,1-dimethylethoxy)carbonyl]amino]-1-(methoxycarbonyl)pentyl]amino]carbonyl]-4-[[[1-[[1,1-dimethylethoxy)carbonyl]-2-methylbutyl]amino]carbonyl]-7-[[[1-[[1,1-dimethylethoxy)carbonyl]-2-methylpropyl]amino]carbonyl]-9,9-dimethyl-9H-xanthen-2-yl]carbonyl]-, 1,1-dimethylethyl ester, stereoisomer (9CI) (CA INDEX NAME)

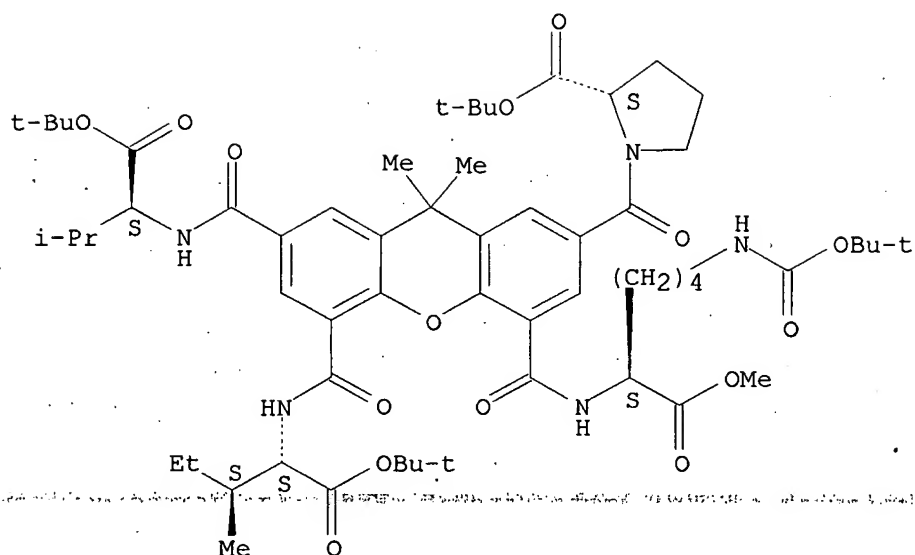
Absolute stereochemistry.



RN 166034-36-2 CAPLUS

CN L-Proline, 1-[[[4-[[[5-[[[1,1-dimethylethoxy)carbonyl]amino]-1-(methoxycarbonyl)pentyl]amino]carbonyl]-5-[[[1-[[1,1-dimethylethoxy)carbonyl]-2-methylbutyl]amino]carbonyl]-7-[[[1-[[1,1-dimethylethoxy)carbonyl]-2-methylpropyl]amino]carbonyl]-9,9-dimethyl-9H-xanthen-2-yl]carbonyl]-, 1,1-dimethylethyl ester, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 12 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:542626 CAPLUS

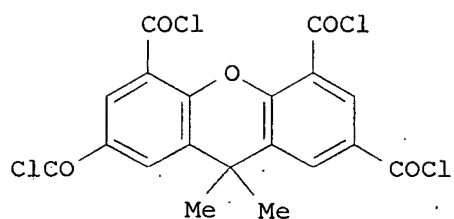
DOCUMENT NUMBER: 123:74100

TITLE: Screening method for isolation in solution of
biologically active compounds from a molecular library
AUTHOR(S): Carell, Thomas; Wintner, Edward A.; Rebek, Julius Jr.
CORPORATE SOURCE: Dep. Chem., Massachusetts Inst. Technol., Cambridge,
MA, 02139, USA

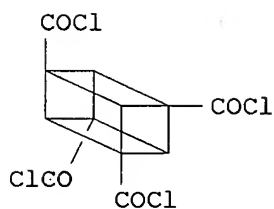
SOURCE: Angewandte Chemie (1994), 106(20), 2162-4, (See also
Angew. Chem., Int. Ed. Engl., 1994, 33(20), 2061-4)
CODEN: ANCEAD; ISSN: 0044-8249

PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: German

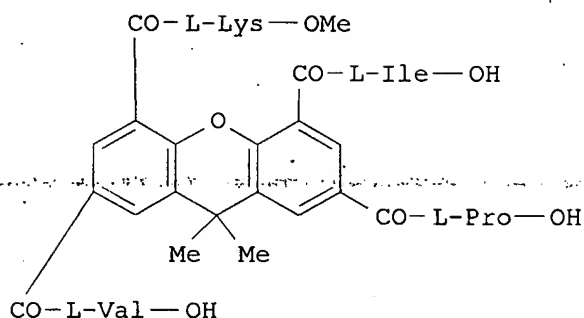
GI



I



II



III

AB I and II were condensed with 19 amino acids to produce a combinatorial library. A method is described whereby this library was screened for trypsin-inhibitory activity. The most active compound in this assay was III.

IT 165465-28-1 165465-29-2

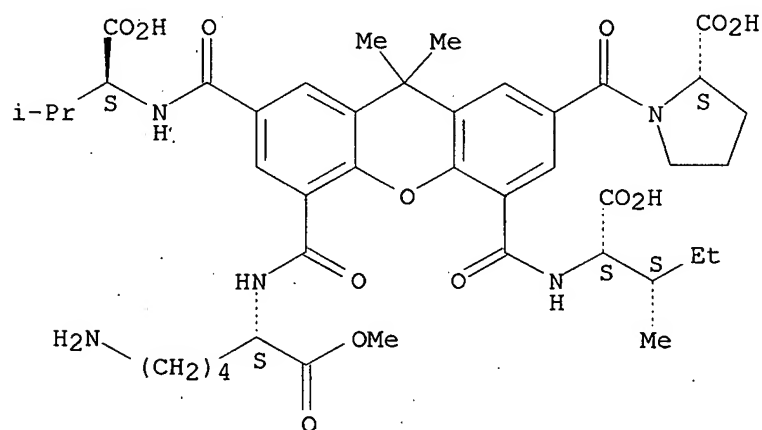
RL: RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)

(reaction products with amino acids; screening method for isolation in solution of biol. active compds. from a mol. library)

RN 165465-28-1 CAPLUS

CN L-Proline, 1-[[5-[[[5-amino-1-(methoxycarbonyl)pentyl]amino]carbonyl]-4-[[[1-carboxy-2-methylbutyl]amino]carbonyl]-7-[[[1-carboxy-2-methylpropyl]amino]carbonyl]-9,9-dimethyl-9H-xanthen-2-yl]carbonyl]-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

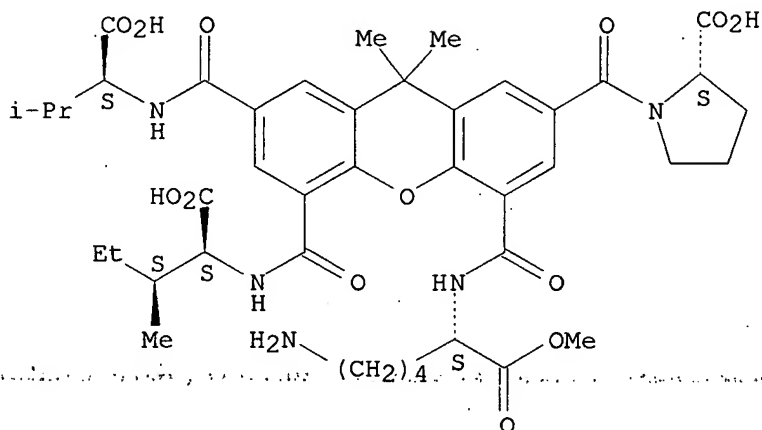


RN 165465-29-2 CAPLUS

CN L-Proline, 1-[[4-[[[5-amino-1-(methoxycarbonyl)pentyl]amino]carbonyl]-5-[[[1-carboxy-2-methylbutyl]amino]carbonyl]-7-[[[1-carboxy-2-

methylpropyl) amino] carbonyl]-9,9-dimethyl-9H-xanthen-2-yl] carbonyl]-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 13 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:107774 CAPLUS

DOCUMENT NUMBER: 120:107774

TITLE: A new class of fluorinated rigid monomers for polyimides

AUTHOR(S): Trofimenko, S.

CORPORATE SOURCE: Exp. Stn., E. I. du Pont de Nemours and Co.,
Wilmington, DE, 19880-0336, USA

SOURCE: Adv. Polyimide Sci. Technol., Proc. Int. Conf.
Polyimides, 4th (1993), Meeting Date 1991, 3-14.
Editor(s): Feger, Claudius; Khojasteh, Mahmoud M.;
Htoo, Maung S. Technomic: Lancaster, Pa.
CODEN: 59CAA2

DOCUMENT TYPE: Conference

LANGUAGE: English

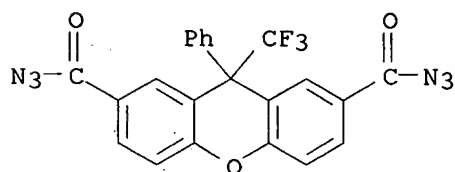
AB A new class of fluorinated monomers for polyimides was developed, based on a 9,9-disubstituted xanthene core, where at least one of the substituents is perfluoroalkyl group. These are exemplified best by 9,9-bis(trifluoromethyl)-2,3,6,7-xanthenetetracarboxylic dianhydride and 9-phenyl-9-trifluoromethyl-2,3,6,7-xanthenetetracarboxylic dianhydride, which were prepared in polymer-grade purity. Other difunctional monomers (diacids, diacyl dichlorides, diisocyanates, diamines, diols) based on the above xanthene cores were also prepared, and the mol. dimensions of these tricyclic cores were determined by means of x-ray crystallog. The scope of perfluoroalkyl and aryl groups usable in this synthesis was explored.

IT 139291-52-4P 152931-32-3P

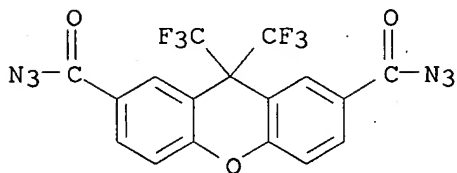
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion to diisocyanate derivative)

RN 139291-52-4 CAPLUS

CN 9H-Xanthene-2,7-dicarbonyl diazide, 9-phenyl-9-(trifluoromethyl)- (9CI)
(CA INDEX NAME)



RN 152931-32-3 CAPLUS
CN 9H-Xanthene-2,7-dicarbonyl diazide, 9,9-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 14 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1993:160556 CAPLUS

DOCUMENT NUMBER: 118:160556

TITLE: Effect of new diamidines against Leishmania donovani infection

AUTHOR(S): Chauhan, P. M. S.; Iyer, R. N.; Shankhdhar, V.; Guru, P. Y.; Sen, A. B.

CORPORATE SOURCE: Med. Chem. Div., Cent. Drug Res. Inst., Lucknow, 226 001, India

SOURCE: Indian Journal of Experimental Biology (1993), 31(2), 196-8

CODEN: IJEBA6; ISSN: 0019-5189

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The impact of interamidine distance on antileishmanial activity of new aryl diamidines have been evaluated against amastigotes of *L. donovani* in hamster. Of the 20 compds. tested, only four (2,8-diamidino-9,10-dihydrodibenzoxepin; 2,7-diamidinioxanthone; 2,7-diamidinethioxanthone and 2,7-diamidinioxanthene) showed significant inhibition (more than 80%) of multiplication of amastigotes in spleen. The interamidine distance in the structure appears to have bearing on antileishmanial activity. The observations made are likely to evoke new understanding on the structure activity relationship of diarylamidines.

IT 146699-20-9, Dibenz[b,f]oxepin-2,8-dicarboximidamide

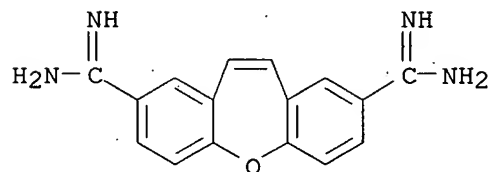
146699-21-0 146699-26-5 146699-28-7,

9H-Xanthene-2,7-dicarboximidamide

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(antileishmanial activity of, structure in relation to)

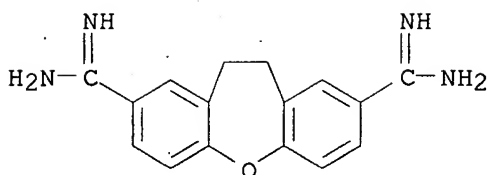
RN 146699-20-9 CAPLUS

CN Dibenz[b,f]oxepin-2,8-dicarboximidamide (9CI) (CA INDEX NAME)

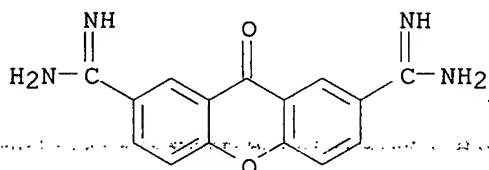


RN 146699-21-0 CAPLUS

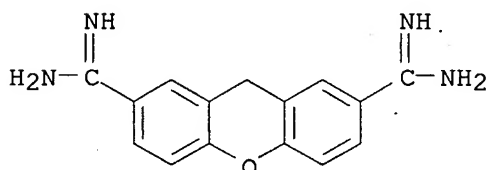
CN Dibenz[b,f]oxepin-2,8-dicarboximidamide, 10,11-dihydro- (9CI) (CA INDEX NAME)



RN 146699-26-5 CAPLUS
CN 9H-Xanthene-2,7-dicarboximidamide, 9-oxo- (9CI) (CA INDEX NAME)



RN 146699-28-7 CAPLUS
CN 9H-Xanthene-2,7-dicarboximidamide (9CI) (CA INDEX NAME)



L4 ANSWER 15 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:102980 CAPLUS
DOCUMENT NUMBER: 118:102980
TITLE: Preparation of polybenzoxazoles, polybenzimidazoles, and polybenzothiazoles
INVENTOR(S): Perry, Robert J.
PATENT ASSIGNEE(S): Eastman Kodak Co., USA
SOURCE: U.S., 12 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5149755	A	19920922	US 1991-726437	19910705
CA 2070269	A1	19930106	CA 1992-2070269	19920602
EP 522469	A2	19930113	EP 1992-111331	19920703
EP 522469	A3	19930929		
R: DE, FR, GB				
JP 05262877	A	19931012	JP 1992-177306	19920706
PRIORITY APPLN. INFO.:			US 1991-726437	A 19910705

AB The polymers are prepared in presence of a catalyst (compds. of Pt, Ni or Pd) and solvent by reaction of CO, aromatic halide X1Ar1Z1, aromatic amine Z2Ar2M1 (X1, Z1, Z2, M1 are non-ortho; one of Z1 and Z2 is X2 and the other is M2; Ar1 and Ar2 are aromatic and heteroarom. 6-20 ring-atom moieties; X1 and X2 are independently I and Br; M1 and M2 are independently moieties having an NH2 group, and ortho to NH2, a group from

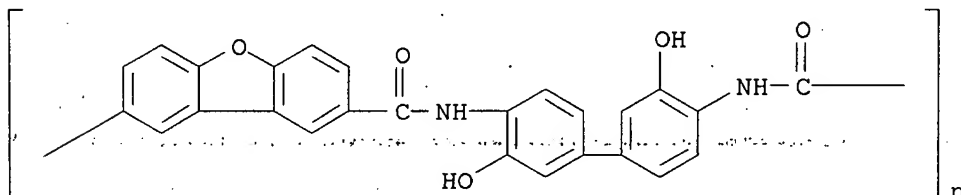
NH₂, OH and SH. Thus, a precyclization polymer was prepared from 4,4'-diiododiphenyl ether, 3,3',4,4'-tetraaminobiphenyl, and CO (7.7 kg/cm²) in AcNMe₂ in presence of bis(triphenylphosphine)palladium(II) chloride/Ph₃P catalyst and base at 120°. Curing to the cyclized polymer was at 100-325°.

IT 146167-65-9P

RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (preparation and cyclization of)

RN 146167-65-9 CAPLUS

CN Poly[2,8-dibenzofurandiylcarbonylimino(3,3'-dihydroxy[1,1'-biphenyl]-4,4'-diyl)iminocarbonyl] (9CI) (CA INDEX NAME)



L4 ANSWER 16 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:448338 CAPLUS

DOCUMENT NUMBER: 117:48338

TITLE: Process for preparation of 2,7-diamidinioxanthene and -thioxanthene

INVENTOR(S): Chauhan, Prem Man Singh; Iyer, Raman Narayan; Shankhdhar, Veena; Guru, Purushottam Yeshwant; Amiya, Bushansen

PATENT ASSIGNEE(S): Council of Scientific and Industrial Research, India

SOURCE: Indian, 7 pp.
CODEN: INXXAP

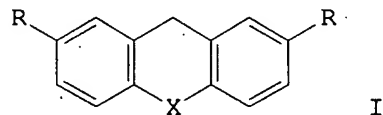
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
IN 167210	A1	19900922	IN 1987-DE626	19870723
PRIORITY APPLN. INFO.: GI			IN 1987-DE626	19870723



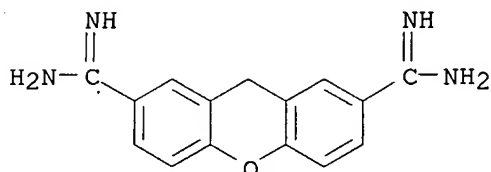
AB Title compds. I (R = H₂NC:NH; X = O, S) useful in treatment of human Kala-azar (no data) are prepared from I (R = Br, X = O, S) by cyanation, hydrolysis, and amination. Thus, I (R = Br, X = S) (preparation given), CuCN, and pyridine were heated to 200° for 48 h to give I (R = NC; X = S) (II). II was treated with HCl/EtOH/dioxane at 0° and the resulting imino ether was treated with EtOH/NH₃ to give I (R = H₂NC:NH, X = S).

IT 112120-90-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as tripanosomicide).

RN 112120-90-8 CAPLUS

CN 9H-Xanthene-2,7-dicarboximidamide, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

L4 ANSWER 17 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:426465 CAPLUS

DOCUMENT NUMBER: 117:26465

TITLE: Platelet aggregation inhibiting and anticoagulant effects of oligoamines. XVII. Oligoamines with fluorescent properties. Part A: fluorescent bridged nitrogen functions

AUTHOR(S): Rehse, K.; Seidel, T.

CORPORATE SOURCE: Inst. Pharm., Freien Univ. Berlin, Berlin, D-1000/33, Germany

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1992), 325(4), 235-9

CODEN: ARPMAS; ISSN: 0365-6233

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

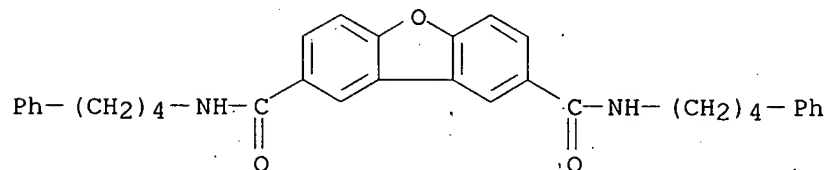
AB Eleven dimethanamines, e.g. acenaphthene derivative I (R = 4-phenylbutyl), phenothiazine derivative II (R = 4-phenylbutyl) and one disydnnonimine III with fluorescent properties were synthesized. All of them show antiplatelet activities (IC₅₀, Born-test) in concns. between 14-75 μmol/L. Five of them inhibited fibrin formation induced by thromboplasmin by more than 75% in a 200 μmolar concentration. The most space consuming fluorophores show the smallest inhibition of the platelet aggregation. The highest activities were obtained with an azulene, acenaphthene or naphthalene moiety between the two basic nitrogen functions.

IT 141914-81-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reduction by lithium aluminum hydride)

RN 141914-81-0 CAPLUS

CN 2,8-Dibenzofurandicarboxamide, N,N'-bis(4-phenylbutyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 18 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:256229 CAPLUS

DOCUMENT NUMBER: 116:256229

TITLE: Derivatives of 9,9-bis(perfluoroalkyl)xanthene and 9-aryl-9-(perfluoroalkyl)xanthene as polymerizable

monomers
 INVENTOR(S): Trofimenko, Swiatoslaw
 PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co., USA
 SOURCE: U.S., 14 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5051520	A	19910924	US 1990-527740	19900523
CA 2042894	A1	19911124	CA 1991-2042894	19910517
EP 458201	A2	19911127	EP 1991-107994	19910517
EP 458201	A3	19930310		
EP 458201	B1	19970827		
R: AT, CH, DE, FR, GB, IT, LI, NL				
AT 157359	T	19970915	AT 1991-107994	19910517
JP 04226973	A	19920817	JP 1991-145234	19910522
JP 3053462	B2	20000619		
US 5097000	A	19920317	US 1991-718936	19910621
US 5101004	A	19920331	US 1991-718935	19910621
US 5153336	A	19921006	US 1991-718937	19910621
US 5202446	A	19930413	US 1991-718932	19910621
PRIORITY APPLN. INFO.:			US 1990-527740	A 19900523

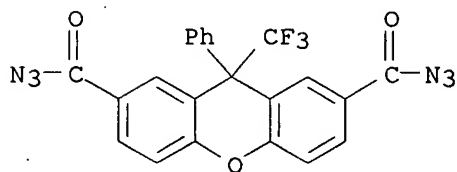
OTHER SOURCE(S): MARPAT 116:256229

AB The title derivs. are prepared and used in the preparation of polyesters, polyimides, etc. Thus, 9,9-bis(trifluoromethyl)-2,3,6,7-xanthenetetracarboxylic dianhydride was prepared and used with bis(4-aminophenyl) ether to prepare a polyimide film having tensile strength 115 MPa, elastic modulus 1.3 GPa, and elongation 21%.

IT 139291-52-4P
 RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (preparation and rearrangement of)

RN 139291-52-4 CAPLUS

CN 9H-Xanthene-2,7-dicarbonyl diazide, 9-phenyl-9-(trifluoromethyl)- (9CI)
 (CA INDEX NAME)



L4 ANSWER 19 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:194158 CAPLUS

DOCUMENT NUMBER: 116:194158

TITLE: Preparation of 2,7-diamidinioxanthone and -thioxanthane as leishmanicides

INVENTOR(S): Chauhan, Prem Man Singh; Iyer, Raman Narayan; Shankhodhar, Veena; Curu, Purushottam Yeshwant; Sen, Amiya Bhushansen

PATENT ASSIGNEE(S): Council of Scientific and Industrial Research, India

SOURCE: Indian, 10 pp.

CODEN: INXXAP

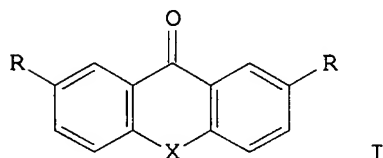
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
IN 167932	A1	19910112	IN 1986-DE373	19860425
PRIORITY APPLN. INFO.:			IN 1986-DE373	19860425
OTHER SOURCE(S):	MARPAT	116:194158		
GI				

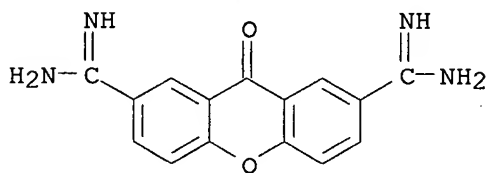


AB Title compds. [I.2HCl; R = C(:NH)NH₂; X = O, S] were prepared as leishmanicides (no data). Thus, I (R = Br, X = O) was heated 24 h with CuCN in pyridine and the product treated sequentially with EtOH/HCl and EtOH/NH₃ to give I.2HCl [R = C(:NH)NH₂, X = O].

IT 112120-88-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as leishmanicide)

RN 112120-88-4 CAPLUS

CN 9H-Xanthene-2,7-dicarboximidamide, 9-oxo-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

L4 ANSWER 20 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1990:431877 CAPLUS

DOCUMENT NUMBER: 113:31877

TITLE: Electrophotographic photoconductor containing disazo pigment

INVENTOR(S): Shiino, Yasuko; Miyazaki, Hajime

PATENT ASSIGNEE(S): Canon K. K., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 17 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01140163	A	19890601	JP 1987-297447	19871127
PRIORITY APPLN. INFO.:			JP 1987-297447	19871127
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title photoconductor, on an elec. conductive substrate, contains a disazo pigment I [A1-2 = (substituted) aromatic cyclohydrocarbon, aromatic heterocycle; A1-2 may be linked by using bonding groups; X1-2 = single bond, O, S, :NR3; R1-2 = (substituted) amido residue, cyclic amido residue, ureido, (cyclic) hydrazido residue; R3 = H, alkyl, aryl]. Thus, on an Al plate, an aqueous NH3 solution of casein was applied, dried, coated with

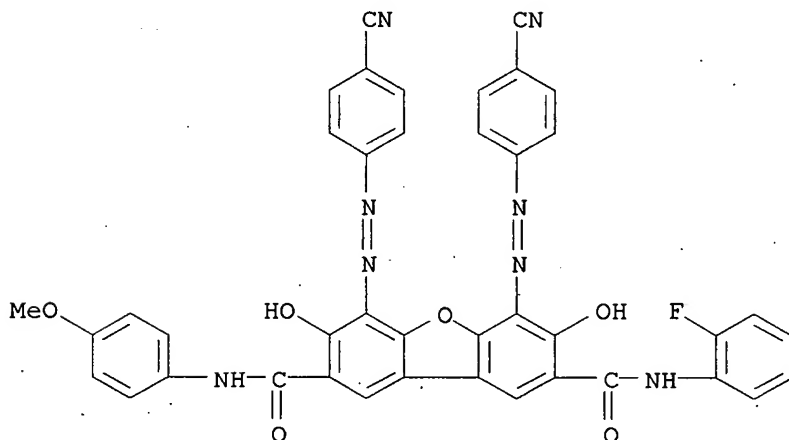
a dispersion comprising disazo pigment II, EtOH, and butyral resin, and overcoated with a hydrazone III solution and poly(Me methacrylate) to give the title photoconductor showing stable elec. potential characteristics under highly-humidity high temperature condition.

IT 125338-66-1

RL: USES (Uses) (pigment, charge-generating layer containing, for electrophotog. photoconductor)

RN 125338-66-1 CAPLUS

CN 2,8-Dibenzofurandicarboxamide, 4,6-bis[(4-cyanophenyl)azo]-N-(2-fluorophenyl)-3,7-dihydroxy-N'-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

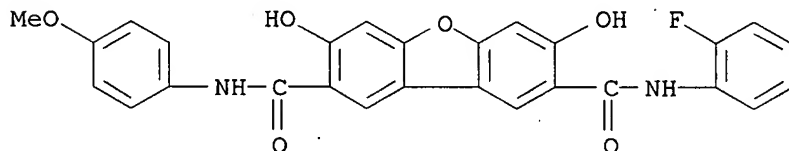


IT 125338-83-2

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, disazo pigment from, for electrophotog. photoconductor)

RN 125338-83-2 CAPLUS

CN 2,8-Dibenzofurandicarboxamide, N-(2-fluorophenyl)-3,7-dihydroxy-N'-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

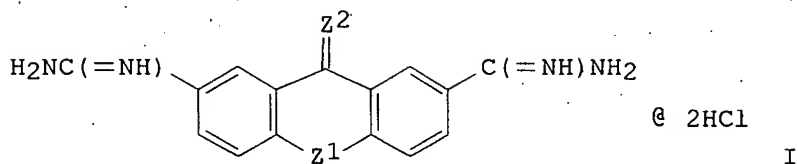


L4 ANSWER 21 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

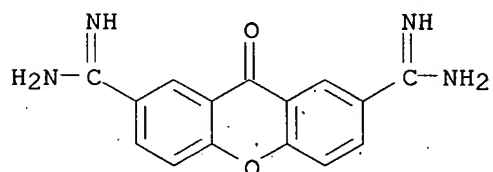
ACCESSION NUMBER: 1988:37591 CAPLUS

DOCUMENT NUMBER: 108:37591

TITLE: Synthesis of 2,7-diamidinioxanthone, thioxanthone and related compounds as potential leishmanicides
 AUTHOR(S): Chauhan, P. M. S.; Rao, K. V. B.; Iyer, R. N.; Shankhadhar, Veena; Guru, P. Y.; Sen, A. B.
 CORPORATE SOURCE: Div. Med. Chem., Cent. Drug Res. Inst., Lucknow, 226 001, India
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1987), 26B(3), 248-50
 CODEN: IJSBDB; ISSN: 0376-4699
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 108:37591
 GI

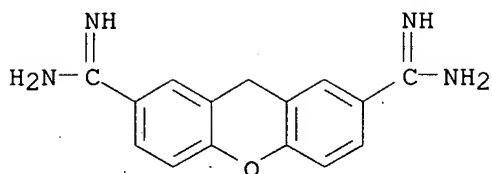


AB Dicarboxamidines I (Z1 = S, O; Z2 = O, H2) were prepared from dibromo compds. via dicarbonitriles. I showed anti-leishmanial and bactericidal activity.
 IT 112120-88-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and anti-leishmanial activity of)
 RN 112120-88-4 CAPLUS
 CN 9H-Xanthene-2,7-dicarboximidamide, 9-oxo-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

IT 112120-90-8P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation and pharmacol. activity of)
 RN 112120-90-8 CAPLUS
 CN 9H-Xanthene-2,7-dicarboximidamide, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

L4 ANSWER 22 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1984:138930 CAPLUS

DOCUMENT NUMBER: 100:138930

TITLE: Synthesis of 2,8-diamidinodibenz[b,f]oxepin and related compounds as potential leishmanicides

AUTHOR(S): Chauhan, P. M. S.; Iyer, R. N.

CORPORATE SOURCE: Med. Chem. Div., Cent. Drug Res. Inst., Lucknow, 226 001, India

SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1983), 22B(9), 898-900

CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 100:138930

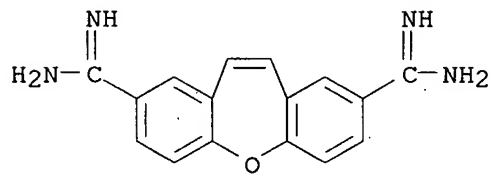
AB 2,8-Diamidinodibenz[b,f]oxepin, the corresponding 10,11-dihydro compound, and [4,2-R(Me)C6H3]2O [R = C(:NH)NH2, C(:NOH)NH2] were prepared from (2-MeC6H4)2O. They have antileishmanial and antimicrobial activity.

IT 89446-94-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and leishmanicidal activity of)

RN 89446-94-6 CAPLUS

CN Dibenz[b,f]oxepin-2,8-dicarboximidamide, dihydrochloride (9CI) (CA INDEX NAME)



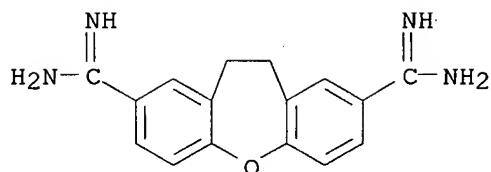
● 2 HCl

IT 89446-93-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 89446-93-5 CAPLUS

CN Dibenz[b,f]oxepin-2,8-dicarboximidamide, 10,11-dihydro-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

L4 ANSWER 23 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1977:433420 CAPLUS

DOCUMENT NUMBER: 87:33420

TITLE: Antiallergic agents. Xanthone-2,7-dicarboxylic acid derivatives.

AUTHOR(S): Jones, Winton D., Jr.; Albrecht, William L.; Munro, Nancy L.; Stewart, Kenneth T.

CORPORATE SOURCE: Merrell-Natl. Lab. Div., Richardson-Merrell Inc., Cincinnati, OH, USA

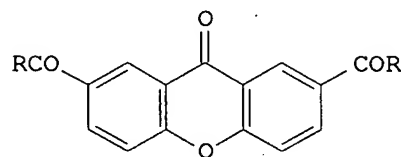
SOURCE: Journal of Medicinal Chemistry (1977), 20(4), 594-5
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 87:33420

GI



I

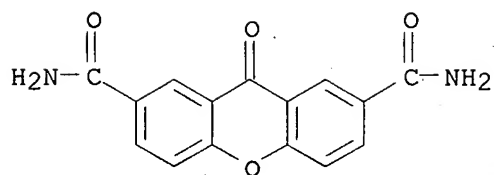
AB Reaction of xanthone-2,7-dicarboxylic acid chloride [40381-96-2] with various amines and N heterocycles gave 11 amides with oral activity as inhibitors of rat passive cutaneous anaphylaxis. I(R = NMe₂) [62032-22-8], the most active compound on a weight basis, inhibited the wheat reaction by 69% at an oral dose of 100 mg/kg. The acid (I, R = OH) and di-Et ester (I, R = OEt) [62032-21-7] had no oral activity. The order of amide oral activity was tertiary > primary > secondary.

IT 62032-13-7P 62032-14-8P 62032-15-9P
62032-16-0P 62032-17-1P 62032-18-2P
62032-19-3P 62032-20-6P 62032-22-8P
62032-37-5P 62066-38-0P

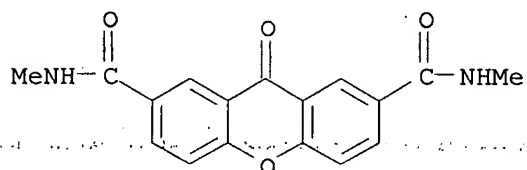
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and immunosuppressant activity of)

RN 62032-13-7 CAPLUS

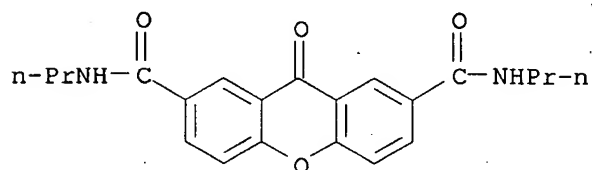
CN 9H-Xanthene-2,7-dicarboxamide, 9-oxo- (9CI) (CA INDEX NAME)



RN 62032-14-8 CAPLUS
 CN 9H-Xanthene-2,7-dicarboxamide, N,N'-dimethyl-9-oxo- (9CI) (CA INDEX NAME)

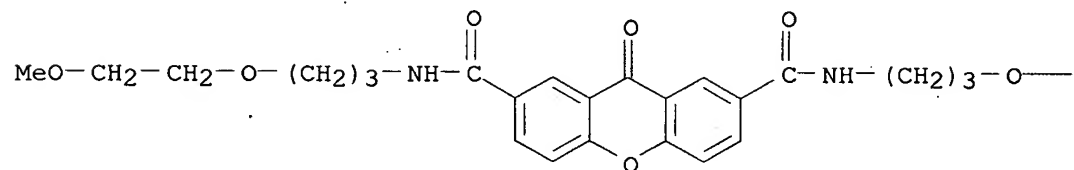


RN 62032-15-9 CAPLUS
 CN 9H-Xanthene-2,7-dicarboxamide, 9-oxo-N,N'-dipropyl- (9CI) (CA INDEX NAME)



RN 62032-16-0 CAPLUS
 CN 9H-Xanthene-2,7-dicarboxamide, N,N'-bis[3-(2-methoxyethoxy)propyl]-9-oxo- (9CI) (CA INDEX NAME)

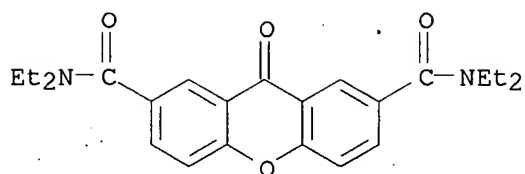
PAGE 1-A



PAGE 1-B

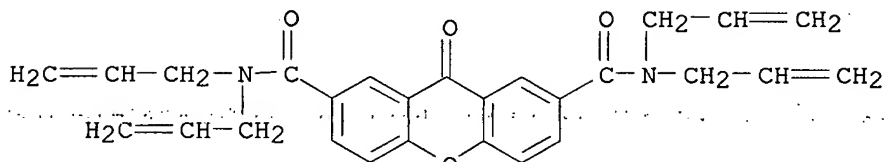
—CH₂—CH₂—OMe

RN 62032-17-1 CAPLUS
 CN 9H-Xanthene-2,7-dicarboxamide, N,N',N',N'-tetraethyl-9-oxo- (9CI) (CA INDEX NAME)



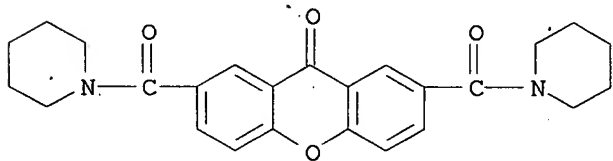
RN 62032-18-2 CAPLUS

CN 9H-Xanthene-2,7-dicarboxamide, 9-oxo-N,N,N',N'-tetra-2-propenyl- (9CI)
(CA INDEX NAME)



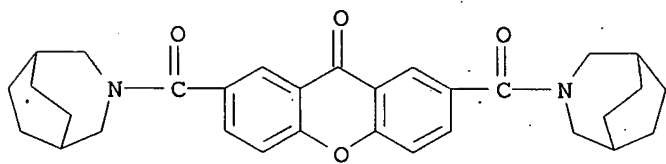
RN 62032-19-3 CAPLUS

CN Piperidine, 1,1'-[(9-oxo-9H-xanthene-2,7-diyl)dicarbonyl]bis- (9CI) (CA
INDEX NAME)



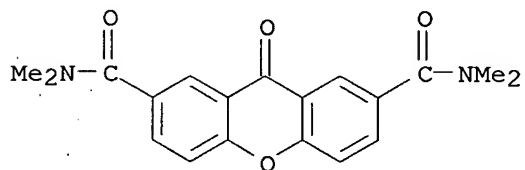
RN 62032-20-6 CAPLUS

CN 3-Azabicyclo[3.2.2]nonane, 3,3'-[(9-oxo-9H-xanthene-2,7-
diyl)dicarbonyl]bis- (9CI) (CA INDEX NAME)



RN 62032-22-8 CAPLUS

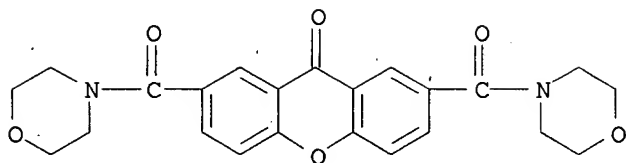
CN 9H-Xanthene-2,7-dicarboxamide, N,N,N',N'-tetramethyl-9-oxo- (9CI) (CA
INDEX NAME)



RN 62032-37-5 CAPLUS

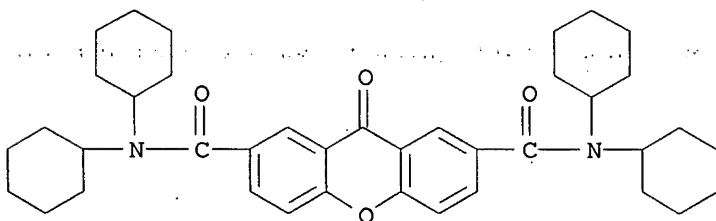
CN Morpholine, 4,4'-[(9-oxo-9H-xanthene-2,7-diyl)dicarbonyl]bis- (9CI) (CA

INDEX NAME)



RN 62066-38-0 CAPLUS

CN 9H-Xanthene-2,7-dicarboxamide, N,N,N',N'-tetracyclohexyl-9-oxo- (9CI) (CA INDEX NAME)



L4 ANSWER 24 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1977:83506 CAPLUS

DOCUMENT NUMBER: 86:83506

TITLE: Bis-basic-substituted polycyclic aromatic compounds. A new class of antiviral agents. 8. Bis-basic derivatives of carbazole, dibenzofuran, and dibenzothiophene

AUTHOR(S): Albrecht, William L.; Fleming, Robert W.; Horgan, Stephen W.; Mayer, Gerald D.

CORPORATE SOURCE: Merrell-Natl. Lab. Div., Richardson-Merrell Inc., Cincinnati, OH, USA

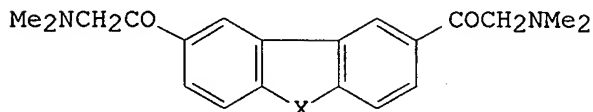
SOURCE: Journal of Medicinal Chemistry (1977), 20(3), 364-71
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 86:83506

GI



I, X=O
2HCl II, X=S

AB A series of 58 bisalkamine esters, bis-basic ethers, bis-basic ketones, aminoalkanes, and carboxamides of carbazole, N-ethylcarbazole, dibenzofuran, and dibenzothiophene was prepared and evaluated in vivo for activity against encephalomyocarditis virus. Within the carbazole and ethylcarbazole series, the bisalkamine esters were most active, while bis-basic ketone derivs. of dibenzofuran and dibenzothiophene were most potent in those series of compds. RMI 11567DA (I) [36115-09-0] and RMI 11877DA (II) [35556-06-0] were active, applied topically, against herpes virus in hairless mice, and induced serum interferon when given orally or s.c. to mice.

IT 30568-74-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and virucidal activity of)

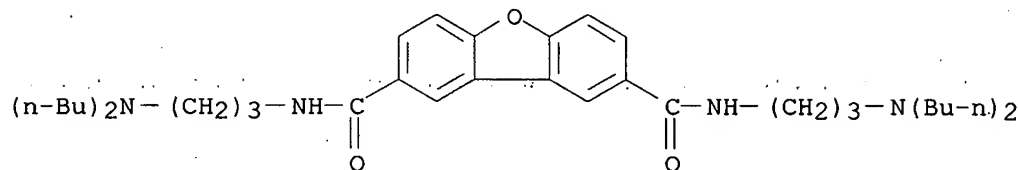
RN 30568-74-2 CAPLUS

CN 2,8-Dibenzofurandicarboxamide, N,N'-bis[3-(dibutylamino)propyl]-, 2-hydroxy-1,2,3-propanetricarboxylate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 47845-67-0

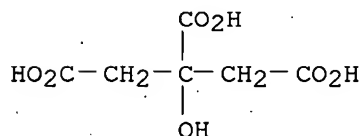
CMF C36 H56 N4 O3



CM 2

CRN 77-92-9

CMF C6 H8 O7



L4 ANSWER 25 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1976:523765 CAPLUS

DOCUMENT NUMBER: 85:123765

TITLE: Antiviral compositions containing bis-basic esters and amides of xanthene and xanthone

INVENTOR(S): Carr, Albert A.; Fleming, Robert W.; Sill, Arthur D.

PATENT ASSIGNEE(S): Richardson-Merrell Inc., USA

SOURCE: U.S., 10 pp. Division of U.S. 3,859,307.

CODEN: USXXAM

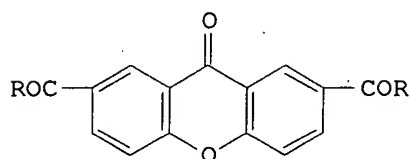
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3957986	A	19760518	US 1973-375754	19730702
US 3859307	A	19750107	US 1971-162716	19710714
IL 39725	A	19760430	IL 1972-39725	19720621
GB 1350520	A	19740418	GB 1972-29594	19720623
CA 976962	A1	19751028	CA 1972-146373	19720705
JP 57025553	B	19820529	JP 1972-68297	19720710
CH 587838	A5	19770513	CH 1972-10370	19720711
FR 2145717	A1	19730223	FR 1972-25600	19720713
NL 7209761	A	19730116	NL 1972-9761	19720714



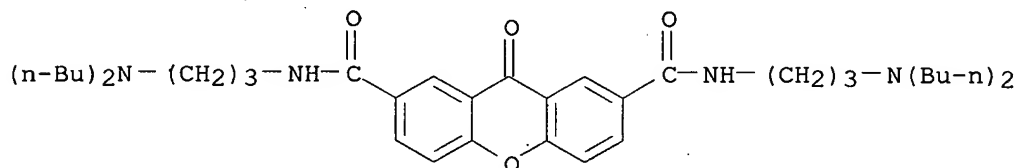
I

AB The xanthonedicarboxylic acid derivs. I [R = O(CH₂)₃NEt₂, O(CH₂)₃NBu₂, NH(CH₂)₃NBu₂] were prepared by chlorinating I (R = OH) and treating I (R = Cl) with the amino alc. or diamine.

IT 40382-01-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 40382-01-2 CAPLUS

CN 9H-Xanthene-2,7-dicarboxamide, N,N'-bis[3-(dibutylamino)propyl]-9-oxo-
(9CI) (CA INDEX NAME)



L4 ANSWER 26 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1976:487090 CAPLUS

DOCUMENT NUMBER: 85:87090

TITLE: Bis-basic-substituted polycyclic aromatic compounds.
A new class of antiviral agents. 7. Bisalkamine
esters of 9-oxoxanthene-2,7-dicarboxylic acid,
3,6-bis-basic ethers of xanthene-9-one, and
2,7-bis(aminoacyl)xanthene-9-ones, -xanthenes, and
-thioxanthenes

AUTHOR(S): Carr, Albert A.; Grunwell, Joyce F.; Sill, Arthur D.;
Meyer, Donald R.; Sweet, F. William; Scheve, B.
Joseph; Grisar, J. Martin; Fleming, Robert W.; Mayer,
Gerald D.

CORPORATE SOURCE: Merrell-Natl. Lab., Div., Richardson-Merrell Inc.,
Cincinnati, OH, USA

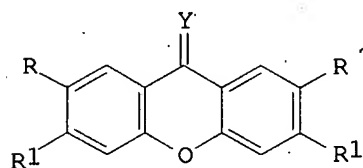
SOURCE: Journal of Medicinal Chemistry (1976), 19(9), 1142-8
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 85:87090

GI



2HCl

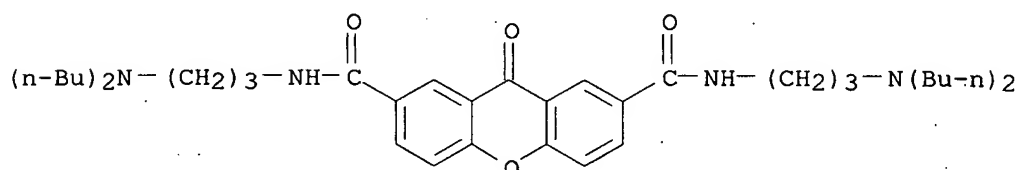
I, R=H, R₁=OCH₂CH₂NMe₂, Y=O
II, R=COCH₂NMe₂, R₁=H, Y=H₂

AB Of 43 title compds., (analog of tilorone [27591-97-5]), prepared and tested against encephalomyocarditis virus infection in mice, about 30 had high activity administered orally or s.c., with bis-basic ether RMI 10874DA-2HCl (I) [54593-27-0] and bisaminoacyl derivative RMI 11513DA-2HCl (II) [37971-99-6] being the most effective of the orally active compds. I and II were also active against RNA arbovirus Semliki Forest virus and vaccinia virus in mice. Structure-activity relations were discussed.

IT 40382-01-2P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation and virucidal activity of)

RN 40382-01-2 CAPLUS

CN 9H-Xanthene-2,7-dicarboxamide, N,N'-bis[3-(dibutylamino)propyl]-9-oxo-
 (9CI) (CA INDEX NAME)



L4 ANSWER 27 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1976:17122 CAPLUS

DOCUMENT NUMBER: 84:17122

TITLE: Bis-basic esters and amides of dibenzofuran

INVENTOR(S): Albrecht, William L.; Fleming, Robert W.

PATENT ASSIGNEE(S): Richardson-Merrell Inc., USA

SOURCE: U.S., 6 pp. Division of U.S. 3,867,409.
 CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3903116	A	19750902	US 1974-512147	19741004
US 3867409	A	19750218	US 1969-833717	19690616
CA 949564	A1	19740618	CA 1970-82659	19700513
GB 1262052	A	19720202	GB 1970-1262052	19700604
IL 34683	A	19740314	IL 1970-34683	19700608
ZA 7004011	A	19710127	ZA 1970-4011	19700612
FR 2052974	A5	19710416	FR 1970-22121	19700616
FR 2052974	A1	19710416		
CH 538470	A	19730815	CH 1970-9109	19700616
JP 51041635	B	19761111	JP 1970-52335	19700616
			US 1969-833717	A3 19690616

PRIORITY APPLN. INFO.:

GI For diagram(s), see printed CA Issue.

AB The title compds. I [R = Et₂NCH₂CH₂CH₂O, Bu₂NCH₂CH₂CH₂O, Me₂NCH₂CH₂CH₂O, (CH₂:CHCH₂)₂NCH₂CH₂CH₂O, Pr₂NCH₂CH₂CH₂O, (Me₂CHCH₂CH₂)₂NCH₂CH₂CH₂O, 3-piperidinopropoxy, Bu₂NCH₂CH₂CH₂NH], possessing antiviral activity, were prepared by condensation of dibenzofuran-2,8-dicarbonyl chloride with RH. I (R = Pr₂NCH₂CH₂CH₂O) increased the survival time of mice inoculated with fatal doses of encephalomyocarditis.

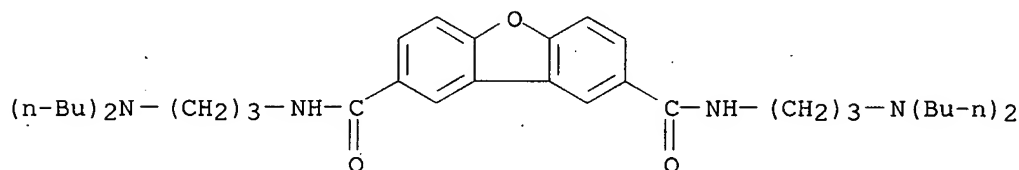
IT' 30568-74-2P.

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)
 RN 30568-74-2 CAPLUS
 CN 2,8-Dibenzofurandicarboxamide, N,N'-bis[3-(dibutylamino)propyl]-,
 2-hydroxy-1,2,3-propanetricarboxylate (1:2) (9CI) (CA INDEX NAME)

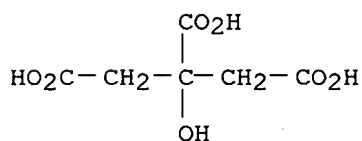
CM 1

CRN 47845-67-0
 CMF C36 H56 N4 O3



CM 2

CRN 77-92-9
 CMF C6 H8 O7



L4 ANSWER 28 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1973:111125 CAPLUS
 DOCUMENT NUMBER: 78:111125
 TITLE: Antiviral bis(aminopropyl) esters and amides of
 xanthene-2,7-dicarboxylates
 INVENTOR(S): Carr, Albert Anthony; Fleming, Robert Willerton; Sill,
 Arthur DeWitt
 PATENT ASSIGNEE(S): Richardson-Merrell Inc.
 SOURCE: Ger. Offen., 34 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2233223	A1	19730201	DE 1972-2233223	19720706
US 3859307	A	19750107	US 1971-162716	19710714
IL 39725	A	19760430	IL 1972-39725	19720621
GB 1350520	A	19740418	GB 1972-29594	19720623
CA 976962	A1	19751028	CA 1972-146373	19720705
JP 57025553	B	19820529	JP 1972-68297	19720710
CH 587838	A5	19770513	CH 1972-10370	19720711
FR 2145717	A1	19730223	FR 1972-25600	19720713
NL 7209761	A	19730116	NL 1972-9761	19720714
PRIORITY APPLN. INFO.:			US 1971-162716	A 19710714

GI For diagram(s), see printed CA Issue.
 AB Four antiviral title compds. (I, X = O or H2, R = Et or Bu, Q = O or NH)

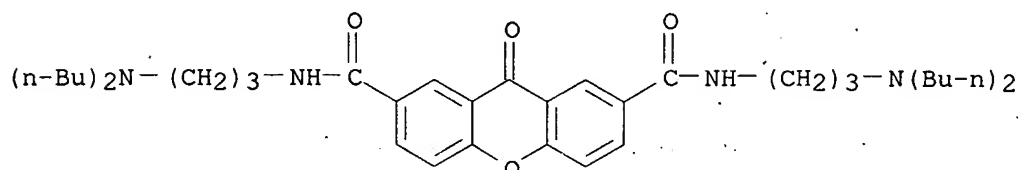
or their dihydrochlorides, applicable in feed, were prepared by esterification or amidation of the corresponding dicarboxylic acids via their chlorides. Thus, refluxing 2,7-xanthenedicarboxylic acid 4 hr with SOCl₂ and pyridine, addition of Bu₂N(CH₂)₃OH in C₆H₆CH₂Cl₂, refluxing 3 hr, and addition of HCl gave 29.6% I.2HCl (X = H₂, Q = O, R = Bu).

IT 40382-01-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 40382-01-2 CAPLUS

CN 9H-Xanthene-2,7-dicarboxamide, N,N'-bis[3-(dibutylamino)propyl]-9-oxo-
(9CI) (CA INDEX NAME)



L4 ANSWER 29 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1971:53504 CAPLUS

DOCUMENT NUMBER: 74:53504

TITLE: Antiviral dibenzofurandicarboxylic acids derivatives

INVENTOR(S): Albrecht, William L.; Fleming, Robert W.

PATENT ASSIGNEE(S): Richardson-Merrell Inc.

SOURCE: Ger. Offen., 22 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2029510	A	19701223	DE 1970-2029510	19700615
DE 2029510	B2	19791004		
DE 2029510	C3	19800619		
US 3867409	A	19750218	US 1969-833717	19690616
CA 949564	A1	19740618	CA 1970-82659	19700513
GB 1262052	A	19720202	GB 1970-1262052	19700604
IL 34683	A	19740314	IL 1970-34683	19700608
ZA 7004011	A	19710127	ZA 1970-4011	19700612
FR 2052974	A5	19710416	FR 1970-22121	19700616
FR 2052974	A1	19710416		
CH 538470	A	19730815	CH 1970-9109	19700616
JP 51041635	B	19761111	JP 1970-52335	19700616
PRIORITY APPLN. INFO.:			US 1969-833717	A 19690616

GI For diagram(s), see printed CA Issue.

AB The title compds. (I) and their salts were prepared and antiviral compns. containing I as active substances were reported. Thus, dibenzofuran-2,8-dicarbonyl chloride was refluxed 12 hr with Et₂N(CH₂)₃OH to give the corresponding I.2HCl [R = O(CH₂)₃NEt₂]. Similarly prepared were 10 I analogs.

IT 30568-74-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

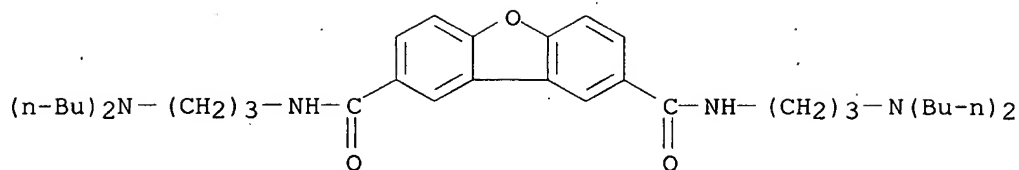
RN 30568-74-2 CAPLUS

CN 2,8-Dibenzofurandicarboxamide, N,N'-bis[3-(dibutylamino)propyl]-,
2-hydroxy-1,2,3-propanetricarboxylate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 47845-67-0

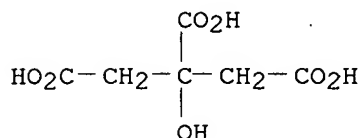
CMF C36 H56 N4 O3



CM 2

CRN 77-92-9

CMF C6 H8 O7



L4 ANSWER 30 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1956:8324 CAPLUS

DOCUMENT NUMBER: 50:8324

ORIGINAL REFERENCE NO.: 50:1663e-i,1664a-h

TITLE: Preparation of aldehydes from carboxylic acids. VI.
Aromatic aldehydes from hydrocarbons through
carboxylic acid N-methylanilides

AUTHOR(S): Weygand, Friedrich; Mitgau, Rotger

CORPORATE SOURCE: Univ. Tübingen, Germany

SOURCE: Chemische Berichte (1955), 88, 301-8

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 50:8324

AB cf. C.A. 49, 15852c. Aromatic hydrocarbons, as well as phenolic ethers, were converted by Friedel-Crafts treatment with PhNMeCOCl (I) and AlCl₃ into ArCONMePh compds. (II, Ar = aryl), which on LiAlH₄ reduction gave the aldehydes. In hydrocarbons with 2 active p-positions, like Ph₂, fluorene, dibenzofuran, were introduced two CONMePh groups, which gave dialdehydes on reduction. Many of the monoaldehydes were known, having been previously prepared by Gattermann-Koch or Gattermann syntheses. The reduction of II with excess LiAlH₄ yielded ArCH₂OH compds. EtOAc (500 g.) saturated with COCl₂ treated dropwise over 1.5-2 h. with 150 g. PhNHMe in 1500 cc. EtOAc while COCl₂ was vigorously introduced, the stream of COCl₂ stopped after addition of the amine, the mixture warmed on the water bath, the EtOAc distilled off, and the residue recrystd. gave 75-85% I, m. 85-6° (from C₆H₆ with C, then from EtOH). (In the following instances many of the aldehydes were isolated as the 2,4-dinitrophenylhydrazone (DNP) to determine the maximum yields at different periods.) I (4.3 g.) treated with 8 cc. PhOMe and 3.7 g. powdered AlCl₃, the mixture warmed to 80-90° in an oil bath, then heated 2 h. at 120°, hydrolyzed with dilute HCl, extracted with Et₂O, the extract dried, the Et₂O and excess PhOMe distilled off, and the residue distilled

gave 4-MeOC₆H₄CONMePh (III), b_{0.02} 154-5°, m. 74° (from

Et₂O), identical (b.p., m.p., and mixed m.p.) with III from 4-MeOC₆H₄COCl and PhNHMe. III (360 mg.) in absolute THF (IIIa) treated with 28 mg. LiAlH₄ 15 h. at 0° afforded 240 mg. p-MeOC₆H₄CHO as the DNP, m. 248° (from AcOH). m-C₆H₄(OMe)₂ (4 g., 15% excess), 4.3 g. I, and 3.7 g. AlCl₃ (10% excess) heated 2.5 h. at 130° in an oil bath, the mixture hydrolyzed, extracted with C₆H₆, the extract dried, evaporated, and the residue

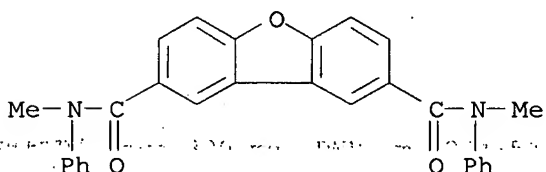
recrystd. yielded 4.0 g. 2,4-HO(MeO)C₆H₃CONMePh (IV), colorless needles, m. 116-17° (from Et₂O). IV (270 mg.) in IIIa treated with 19 mg. LiAlH₄ 2-3 h. at 0° gave 245 mg. DNP, m. 256° (from xylene), of 2,4-HO(MeO)C₆H₃CHO, m. 39°, (obtained from 2.57 g. IV in 40 cc. absolute IIIa with 270 mg. LiAlH₄). I (4.6 g.), 3.6 g. PhOH, and 5.5 g. AlCl₃ heated 2 h. at 100-20° in an oil bath and worked up like IV gave 5.5 g. PhO₂CNMePh (V), m. 57-8° (from C₆H₆), which did not undergo Fries rearrangement. V (227 mg.) reduced as above with 26 mg. LiAlH₄ gave 146 mg. DNP, m. and mixed m. 160-1° of HCHO. PhMe (6 cc.), 4.3 g. I, and 4 g. AlCl₃ heated 5 h. at 110-25° gave 3 g. 4-Me-C₆H₄CONMePh (VI), m. 70° (from Et₂O-petr. ether). VI (335 mg.) reduced 10 h. with 30 mg. LiAlH₄ at 0° gave 300 mg. DNP, m. 234-5°, of 4-MeC₆H₄CHO. m-Xylene (6 cc.), 4.3 g. I, and 4 g. AlCl₃ heated 3 h. at 90-120° gave 2.5 g. 2,4-Me₂C₆H₃CONMePh (VII), m. 49-50° (from petr. ether). VII (240 mg.) treated with 19 mg. LiAlH₄ 1-4 h. at 0° yielded 159-65 mg. DNP, m. 221-2° (from PhMe) of 2,4-Me₂C₆H₃CHO. Similar treatment of 6 cc. o-xylene 2.5 h. at 100-30° gave 3.6 g. 3,4-Me₂C₆H₃CONMePh (VIII), m. 75-6°, reduced as above to 3,4-Me₂C₆H₃CHO [DNP, m. 231° (from xylene)]. VIII (2.39 g.) in 40 cc. IIIa treated gradually with cooling with 260 mg. LiAlH₄, refluxed 6 h., MeOH added, then dilute H₂SO₄, the mixture extracted with

Et₂O, the extract dried, evaporated, and the residual solid (1.30 g.) crystallized

gave 3,4-Me₂C₆H₃CH₂OH, m. 61-2° (from petr. ether). From p-xylene was obtained, 62% 2,5-Me₂C₆H₃CONMePh (IX), m. 70-1° (from petr. ether), reduced to 55-7% 2,5-Me₂C₆H₃CHO [DNP, m. 214-15° (from PhMe)]; with excess LiAlH₄, IX gave 90% 2,5-Me₂C₆H₃CH₂OH [phenylurethane, m. 85-6° (from petr. ether)]. Pseudocumene gave 2,4,5-Me₃C₆H₂CONMePh, light yellow oil, b_{0.01} 138°, reduced to 46% 2,4,5-Me₃C₆H₂CHO, [DNP, m. 212-14° (from xylene)]. Mesitylene gave, in good yield, 2,4,6-Me₃C₆H₂CONMePh b_{0.003} 135-6°, which, because of steric effects, could not be reduced to the aldehyde. Ph₂ gave 83.5% 4-PhC₆H₄CONMePh (X), m. 107° (from ligroine and some alc.), reduced to 4-PhC₆H₄CHO (63% yield after 4 h., 70% after 8 h.) [DNP, m. 236° (from PhMe)]. X gave 75% 4-PhC₆H₄CH₂OH, m. 102° (from petr. ether). From Ph₂ was also obtained 55% (4-PhMeNCOC₆H₄)₂ (XI), m. 227-8° (from ligroine), mixed m.p. undepressed with XI prepared by a Schotten-Baumann reaction of (4-ClOCC₆H₄)₂ and PhNHMe. Reduction of XI gave 68-9% of the dialdehyde, [bis-DNP, m. above 300° (crystallizing poorly from pyridine)]. XI with excess LiAlH₄ afforded 79% (4-HOCH₂C₆H₄)₂, m. 188-9°. Fluorene (XII) gave 60% N-methyl-2-fluorene-carboxanilide (XIII), m. 124-5° (from Et₂O), hydrolyzed to 2-fluorene-carboxylic acid, m. 274°, with KOH in MeOH. XIII gave after 14-20 h. 55-60% 2-fluorene-carboxaldehyde [DNP, m. 259-60° (from xylene)]. XII also gave 37% N,N'-dimethyl-2,7-fluorenedicarboxanilide (XIV), m. 215° (from IIIa and Et₂O). XIV afforded 54% corresponding dialdehyde, isolated as the bis-DNP, m. above 300°. Dibenzofuran (XV) gave 80% (crude) N-methyl-3-dibenzofurancarboxanilide (XVI), m. 126-7° (anal. sample from Et₂O), hydrolyzed with KOH in MeOH to 3-dibenzofurancarboxylic acid, m. 248-9° (from EtOH). XVI gave 69-74% 3-dibenzofurancarboxaldehyde [DNP, m. 286° (decomposition) (crystallizing poorly from xylene-pyridine)]. XVI with excess LiAlH₄ yielded 3-dibenzofuran-methanol, m. 124° (from Et₂O). XV also gave 44% N,N'-dimethyl-3,6-dibenzofurandicarboxanilide, m. 195° (anal. sample from EtOH), reduced to 58-63% of the corresponding dialdehyde

[bis-DNP, m. above 360° (from pyridine)]. C₁₀H₈ yielded 1-C₁₀H₇CONMePh, m. 113° (from EtOH), identical with material prepared from 1-C₁₀H₇COCl and PhNHMe. From 2-H₂NC₆H₄CONMePh, was obtained 55% 2-H₂NC₆H₄CHO [DNP (XVII), m. 244° (decomposition) (from pyridine-EtOH), identical with material obtained by FeSO₄ reduction of 2-O₂NC₆H₄CHO and conversion of the H₂N compound to XVII, m. 244° (decomposition)].

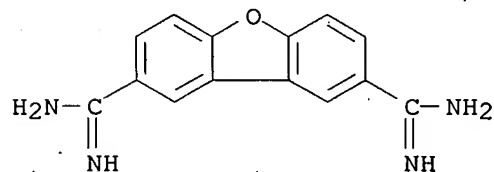
IT 667941-14-2P, 2,8-Dibenzofurandicarboxanilide, N,N'-dimethyl-
 RL: PREP (Preparation)
 (preparation of)
 RN 667941-14-2 CAPLUS
 CN 2,8-Dibenzofurandicarboxanilide, N,N'-dimethyl- (5CI) (CA INDEX NAME)



L4 ANSWER 31 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1951:52867 CAPLUS
 DOCUMENT NUMBER: 45:52867
 ORIGINAL REFERENCE NO.: 45:9027g-h
 TITLE: 3,6-Diamidinodibenzofuran
 AUTHOR(S): Moffatt, J. S.
 CORPORATE SOURCE: Univ. Glasgow, UK
 SOURCE: Journal of the Chemical Society (1951) 625-6
 CODEN: JCSOA9; ISSN: 0368-1769
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

AB A mixture of 5.5 g. 3,6-dibromodibenzofuran and 6.5 g. CuCN, added in small portions to 20 g. boiling quinoline and refluxed 30 min., gives 2.9 g. of the dicyanide (I), m. 299°. I (2.8 g.) in 45 cc. anhydrous EtOH at 0°, saturated with dry HCl and kept 14 days at room temperature, gives 2.8 g. 3,6-guanyldibenzofuran-2HCl.2H₂O, m. above 320°. Subcutaneous injections of doses approaching the maximum tolerated cure infections of Trypanosoma congolense and T. brucei in mice.

IT 232940-74-8P, 2,8-Dibenzofurandicarboxamidine, dihydrochloride
 RL: PREP (Preparation)
 (preparation of)
 RN 232940-74-8 CAPLUS
 CN 2,8-Dibenzofurandicarboximidamide, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

L4 ANSWER 32 OF 32 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1951:52866 CAPLUS
 DOCUMENT NUMBER: 45:52866

ORIGINAL REFERENCE NO.: 45:9027a-g
TITLE: The synthesis of substituted penicillins and simpler structural analogs. I. α -Amino monocyclic β -lactams
AUTHOR(S): Sheehan, John C.; Ryan, James J.
CORPORATE SOURCE: Massachusetts Inst. Technol., Cambridge
SOURCE: Journal of the American Chemical Society (1951), 73, 1204-6
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 45, 4682a. α -C₆H₄(CO)NCH₂COCl (4.48 g.) in 40 cc. C₆H₆ added dropwise during 30 min. to 7.24 g. PhCH:NPh and 2.77 cc. Et₃N in 70 cc. C₆H₆, the mixture stirred 1 hr., the product filtered off, washed with water, filtered, the residue discarded, the C₆H₆ filtrate and the wash water concentrated in vacuo, the semi-solid digested with three 30-cc. portions of 1:1 Et₂O-petr. ether, and the residue extracted with 200 cc. boiling EtOH 30 min., and filtered yielded 3.68 g. 1,4-diphenyl-3-phthalimido-2-azetidinone (I); fine colorless rods with 0.5 mol. dioxane from 1:1 dioxane-water, m. 230-1°; unsolvated I m. 230.5°. I (1 g.), 2.8 cc. M N₂H₄.H₂O in EtOH, and 25 cc. EtOH refluxed 2 hrs., the solution allowed to stand overnight, dried in vacuo, the residue stirred 2 hrs. with 25 cc. 5 N HCl, filtered, and the solid extracted with two 25-cc. portions of water yielded 0.41 g. α -C₆H₄(CO)N₂NH₂; the combined acid and aqueous exts. plus 3 cc. concentrated HCl yielded (after 2 hrs.) 0.40

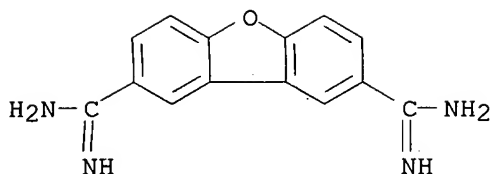
g. 3-amino-1,4-diphenyl-2-azetidinone-HCl (II), colorless rectangular prisms, m. 237.5° (decomposition); free base, m. 118-19° after sintering at 110° (probably a hydrate). PhCH₂COCl (0.062 g.) in 5 cc. CH₂Cl₂ added to 10 cc. CH₂Cl₂ containing 0.110 g. II and 0.064 g. pyridine, the solution concentrated to 7 cc., washed with the following 5-cc. portions, 2 of water, 1 of 0.01 N HCl, 2 of water, 2 of 5% NaHCO₃, and 2 of water, the solution filtered through paper wet with CH₂Cl₂, the filtrate concentrated in air to 1.5 cc., 1 cc. Et₂O added, and the precipitate centrifuged yielded 0.80 g. 1,4-diphenyl-3-(α -phenylacetamido)-2-azetidinone (III), m. 199.5-200° (sintering at 194°) (from 2:1 Me₂CO-water). Dry HCl passed into 0.255 g. II in 25 cc. absolute MeOH for 4 hrs., the stoppered flask stored overnight, and the solution refluxed, filtered, and concentrated

to near dryness yielded 0.22 g. Me α -amino- β -anilino- β -phenylpropionate-2 HCl, m. 140.5-41° (evolution of gas). I (0.40 g.) refluxed 16 hrs. in 25 cc. 0.1 N NaOH yielded 0.17 g. β -anilino- β -phenyl- α -(α -carboxybenzamido)propionic acid, m. 137.5-8.5° (decomposing from 130°). (MeSO₂)₂NCH₂COCl (2.00 g.) in 50 cc. C₆H₆ added dropwise (20 min.) to 3.00 g. PhCH:NPh and 1.11 cc. Et₃N in 15 cc. C₆H₆, and the viscous mixture stirred manually for 30 min. and filtered yielded 1.22 g. 1,4-diphenyl-3-[(dimethanesulfonyl)amino]-2-azetidinone, fine colorless needles from 2:1 Me₂CO-water, m. 235.5-6.5°. 3,1,2-O₂NC₆H₃(CO)NCH₂COCl (2.69 g.) in 55 cc. warm C₆H₆ added dropwise to 3.62 g. PhCH:NPh and 1.39 cc. Et₃N in 10 cc. C₆H₆ during 1 hr., and the mixture allowed to stand 16 hrs. and processed as for I yielded 2.66 g. 1,4-diphenyl-3-(3-nitrophthalimido)-2-azetidinone (IV), crystals with 1 mol. solvent from C₆H₆, m. 163-6° (evolution of gas). IV is polymorphic. The m.p. varies with the recrystn. solvent.

IT 232940-74-8P, 2,8-Dibenzofurandicarboxamidine, dihydrochloride
RL: PREP (Preparation)
(preparation of)

RN 232940-74-8 CAPLUS

CN 2,8-Dibenzofurandicarboximidamide, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

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(FILE 'HOME' ENTERED AT 06:26:04 ON 19 JUL 2007)

FILE 'REGISTRY' ENTERED AT 06:26:13 ON 19 JUL 2007

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 82 S L1 FULL

FILE 'CAPLUS' ENTERED AT 06:26:51 ON 19 JUL 2007

L4 32 S L3 FULL

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COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
186.50	358.81

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-24.96	-24.96

CA SUBSCRIBER PRICE

STN INTERNATIONAL LOGOFF AT 06:49:27 ON 19 JUL 2007